A new perturbative expansion of the time evolution operator associated with a quantum system

P. Aniello *

Istituto Nazionale di Fisica Nucleare, Sezione di Napoli,
and
Dipartimento di Scienze Fisiche dell'Università di Napoli "Federico II",
Complesso Universitario di Monte S. Angelo, Via Cintia - 80126 Napoli, Italy

1st February 2008

Abstract

A novel expansion of the evolution operator associated with a – in general, time-dependent – perturbed quantum Hamiltonian is presented. It is shown that it has a wide range of possible realizations that can be fitted according to computational convenience or to satisfy specific requirements. As a remarkable example, the quantum Hamiltonian describing a laser-driven trapped ion is studied in detail.

Keywords: evolution operator, time-dependent perturbation theory, Magnus expansion.

1 Introduction

The explicit determination of the evolution operator associated with a quantum system — namely, the determination of its explicit action on the state vectors, or, equivalently, on a given orthonormal basis — is, in general, a 'touchy business'. If the Hamiltonian of the system does not depend on time and has the form of the sum of a solvable unperturbed Hamiltonian plus an analytic perturbation, one can use the tools of standard perturbation theory [1] for linear operators, based on the expansion of the resolvent, in order to get approximate expressions of the evolution operator. Alternatively, one can apply a suitable operator perturbative approach [2, 3, 4, 5, 6] in order to obtain a very convenient perturbative expansion of the evolution operator whose truncations have the remarkable property of forming one-parameter groups of unitary operators. The main goal of this paper is to extend, in a natural way, such a perturbative approach to the general case where the quantum Hamiltonian may depend on time.

* Paolo.Aniello@na.infn.it

We stress that if a quantum Hamiltonian is time-dependent — i.e. it describes a non-isolated quantum system — the task of determining the associated time evolution operator is a tough problem since, whenever the values of the Hamiltonian at different times do not commute, the evolution operator does not admit a simple formal expression.
In two fundamental papers [7], Dyson developed an expansion of the evolution operator that has been adopted extensively in any field of physics. Dyson expansion has a transparent physical interpretation in terms of time ordered elementary processes which makes its application particularly appealing, especially in quantum field theory. On the other hand, for many applications, Dyson expansion has severe drawbacks, as a low convergence rate and the lack of unitarity of its truncations [8].
Later, Magnus [9] introduced an expansion of the evolution operator such that each of its truncations retains the property of being unitary. Magnus expansion has been 're-discovered' and re-elaborated several times, and applied successfully to several problems (see [10] and references therein). It is written in the form of the exponential of the expansion of a suitable time-dependent anti-hermitian operator which can be deduced, order by order, from the Hamiltonian of the system. Now, precisely for this reason — just like for the evolution operator generated by a time-independent Hamiltonian — the problem of *computing* explicitly the action of (any truncation of) the Magnus expansion on the state vectors is non-trivial. Truncating the power expansion of the exponential would lead to non-unitary expressions, thus to the loss of the most important feature of Magnus expansion. Besides, in the important case of a time-independent Hamiltonian, there is no link between Rayleigh-Schrödinger-Kato perturbation theory for linear operators and Magnus expansion, a clue suggesting that the power of the perturbative approach is not 'fully exploited' by this expansion.
Then, the issue of finding a generalization of Magnus expansion retaining the property of having unitary truncations, but allowing more convenient solutions — or solutions having special properties — arises in a natural way. In the present paper, we have tried to achieve this result. We introduce a perturbative decomposition of the evolution operator that generalizes Magnus expansion, and opens the possibility of obtaining computational advantages and of satisfying specific requirements for the perturbative solutions by suitably fixing, at each perturbative order, certain arbitrary operators or operator-valued functions. It is important to remark that, in the case where the Hamiltonian does not depend on time, our decomposition, differently from Magnus expansion, assumes a special meaning and has a precise link with standard perturbation theory for linear operators.
The idea of generalizing Magnus expansion is not completely new. It appears in a paper by Casas *et al.* [11] in which the authors introduce the *Floquet-Magnus expansion* for the evolution operator associated with a (interaction picture) Hamiltonian depending periodically on time. However, it turns out that our approach generalizes the one proposed by Casas *et al.* even in the case where the interaction picture Hamiltonian is periodic on time.

We have made the choice of skipping, as far as possible, mathematical complications. Our choice is motivated by various reasons. First, we believe that heuristic investigation should always precede rigorous re-elaboration. Once that it is clear what the basic 'rules of the game' are, one can adopt the most appropriate mathematical tools. Moreover, we avoid the risk of hiding in a thick cloud of technicalities the main ideas and of discouraging

those who may want to *apply* our method for solving problems. It should be also observed that a recent trend in quantum mechanics is to focus on systems which can be described by effective Hamiltonians in finite-dimensional Hilbert spaces (consider the huge research area related to quantum computation and quantum information theory; see ref. [12] and the rich bibliography therein). The study of these systems is not affected by the technicalities associated with the infinite-dimensional spaces but retains all the most intriguing features of quantum physics.
The structure of the paper is the following. We begin introducing, in sect. 2, before going through the details of a our perturbative approach, a significant example — the quantum Hamiltonian describing a laser-driven trapped ion — example that will play a double role: a starting motivation for our analysis and a concrete playing field for practising our theoretical results. In sect. 3 we establish the general form of the perturbative decomposition of the evolution operator that we propose. In the subsequent two sections, we pursue the task of finding a recursive procedure that allows to compute, order by order, the various terms of our perturbative expansion. Precisely: in sect. 4 we study the case where the Hamiltonian does not depend on time and investigate the link with standard perturbation theory for linear operators; in sect. 5 we consider the general case of a time-dependent Hamiltonian. Next, sect. 6 is devoted to study in detail the significant example introduced in sect. 2, in such a way to illustrate the main features of our perturbative expansion of the evolution operator. Finally, in sect. 7, conclusions are drawn, with a quick glance to further applications.

2 A remarkable example: the ion trap Hamiltonian

Before introducing our perturbative approach, we think that is worth considering first a remarkable example: the Hamiltonian describing a one-dimensional laser-driven ion trap. The study of this Hamiltonian, which will be performed systematically in sect. 6, allows to illustrate in a simple way all the main points of the theory developed in the subsequent sections.

A two-level ion of mass μ in a potential trap, with strong confinement along the y and z axes, and weak harmonic binding of frequency ν along the x-axis (the 'trap axis'), can be described — neglecting the motion of the ions transverse to the trap axis — by a Hamiltonian of the following type ($\hbar = 1$):

$$H_0 = \nu\,\hat{n} + \frac{1}{2}\,\epsilon\,\sigma_z\,,$$

where $\hat{n} = a^\dagger a$ is the 'number operator' — with a denoting the vibrational annihilation operator

$$a = \left(\frac{\mu\,\nu}{2}\right)^{\frac{1}{2}} \left(\hat{x} + \frac{i}{\mu\,\nu}\,\hat{p}_x\right)$$

— and σ_z the effective spin operator associated with the internal degrees of freedom of the ion. Let us suppose now that the ion is addressed by a laser beam of frequency α in

a 'traveling wave configuration'. Then, the Hamiltonian describing the physical system becomes (see, for instance, ref. [13]):

$$H_0 + H_\updownarrow(t)\,, \tag{1}$$

where the time-dependent interaction term $H_\updownarrow(t)$ is defined by

$$H_\updownarrow(t) := \Omega_R \left(e^{i\alpha t}\, D(i\eta)^\dagger\, \sigma_- + e^{-i\alpha t}\, D(i\eta)\, \sigma_+ \right), \tag{2}$$

with Ω_R denoting the Rabi frequency (which is proportional to the intensity of the laser field) and with $\sigma_\pm := |\pm\rangle\langle\mp|\,,\ \sigma_+ = \sigma_-^\dagger\ \ (\sigma_z\,|\pm\rangle = \pm\,|\pm\rangle)$. Moreover, we have set:

$$D(i\eta) := \exp\left(i\eta \left(a + a^\dagger \right) \right), \tag{3}$$

where

$$\eta := \frac{k_L \cos\phi}{\sqrt{2\mu\nu}} \tag{4}$$

— with $\mathbf{k}_L$ the wavevector and ϕ the angle between the x-axis and $\mathbf{k_L}$ — is the so-called 'Lamb-Dicke parameter'. In the case where $\eta \ll 1$ ('Lamb-Dicke regime') — a case often occurring in applications[1] — one can keep only those terms in the power expansion of $D(i\eta)$ which are at most linear in η:

$$H_\updownarrow(t) \approx \Omega_R \left(e^{i\alpha t}\, (1 - i\eta(a + a^\dagger))\, \sigma_- + \ h.c. \right) =: H_{\updownarrow}(t)\,. \tag{5}$$

Observe that the problem of dealing with the time-dependent Hamiltonian $H_0 + H_\updownarrow(t)$ can be bypassed by switching to the interaction picture with reference Hamiltonian $\frac{1}{2}\,\alpha\,\sigma_z$. Indeed, setting

$$R_t := \exp\left(-\frac{i}{2}\,\alpha\,\sigma_z\,t \right), \tag{6}$$

one obtains the time-independent 'rotating frame Hamiltonian'

$$\begin{aligned} R_t^\dagger \left(H_0 + H_\updownarrow(t) - \frac{1}{2}\,\alpha\,\sigma_z \right) R_t \ &= \ \nu\,\hat{n} + \frac{1}{2}\,\delta\,\sigma_z + \Omega_R \left(D(i\eta)^\dagger\,\sigma_- + D(i\eta)\,\sigma_+ \right) \\ \text{(Lamb-Dicke regime: } \eta \ll 1) \qquad &\approx \ \Omega_R \left((1 - i\eta(a + a^\dagger))\,\sigma_- + \ h.c. \right), \end{aligned} \tag{7}$$

where $\delta := \epsilon - \alpha$ is the ion-laser detuning. In many applications, the condition $\Omega_R \ll \nu$ is also verified; hence, it is natural to introduce the (dimensionless) perturbative parameter

$$\lambda \equiv \frac{\Omega_R}{\nu} \ll 1\,. \tag{8}$$

[1] Notice that in a trap with a *linear geometry*, like the one we are considering here, one can modify the incidence angle ϕ of the laser beam with respect to the principal axis of the trap in order to control the Lamb-Dicke parameter η.

Thus, the study of the time-dependent Hamiltonian (1) can ultimately be reduced to the study of the simpler time-independent Hamiltonian

$$\bar{H} := \nu\,\hat{n} + \frac{1}{2}\,\delta\,\sigma_z + \lambda\,\nu\left((1 - i\eta(a + a^\dagger))\,\sigma_- + \ h.c.\right), \tag{9}$$

which has the form of a trivially solvable Hamiltonian[2] $\bar{H}_0 := \nu\,\hat{n} + \frac{1}{2}\,\delta\,\sigma_z$ plus a 'small perturbation' $\bar{H}_\updownarrow := \lambda\,\nu\left((1 - i\eta(a + a^\dagger))\,\sigma_- + \ h.c.\right)$.

The exact eigenvalues and eigenprojectors of the Hamiltonian $\bar{H}$, despite its formal simplicity, are not known. Hence, at this point, it would seem reasonable to adopt a (time-independent) perturbative approach for studying the Hamiltonian $\bar{H}$. However, this is not what it is usually done in the literature. In fact, with the aim of providing an approximate expression of the evolution operator associated with the Hamiltonian $\bar{H}$, the *rotating wave approximation* (RWA) — see, for instance, ref. [14] — is usually applied. This approximation amounts to passing to a further interaction picture with reference Hamiltonian $\bar{H}_0$, so obtaining the new interaction picture Hamiltonian

$$\bar{H}_{\rm int}(t) = \lambda\,\nu\left(1 - i\eta(e^{i\nu t}\,a^\dagger + e^{-i\nu t}\,a)\right)e^{-i\delta t}\,\sigma_- + \ h.c.$$

— which is once again time-dependent like the ion trap Hamiltonian (1) — and, then, retaining only those terms in $\bar{H}_{\rm int}(t)$ which are 'slowly rotating'; all the other terms, often called 'counter-rotating terms' (for historical reasons), are simply ignored.
In particular, in correspondence to the three types of *resonance condition*

$$\delta = \epsilon - \alpha \approx 0\,, \quad \delta + \nu \approx 0\,, \quad \delta - \nu \approx 0\,, \tag{10}$$

one obtains, respectively, the following three types of effective interaction picture Hamiltonian:

$$\bar{H}^{(0)}_{\rm eff} \ = \ \lambda\,\nu\,(\sigma_- + \ \sigma_+)\,, \qquad\qquad (\,\delta \approx \ 0\,) \tag{11}$$

$$\bar{H}^{(-)}_{\rm eff} \ = \ i\,\lambda\,\nu\,\eta\left(a^\dagger\,\sigma_+ - \ a\,\sigma_-\right), \qquad (\,\delta \approx -\nu\,) \tag{12}$$

$$\bar{H}^{(+)}_{\rm eff} \ = \ i\,\lambda\,\nu\,\eta\left(a\,\sigma_+ - \ a^\dagger\,\sigma_-\right). \qquad (\,\delta \approx +\nu\,) \tag{13}$$

These effective Hamiltonians, in correspondence to the respective resonances, commute with the reference Hamiltonian $\bar{H}_0$. This is due to the fact that the resonances (10) are associated with the appearance of *degeneracies* in the spectrum of the reference Hamiltonian, and the degenerate eigenspaces of $\bar{H}_0$ are invariant subspaces for the effective Hamiltonians $\bar{H}^{(0)}_{\rm eff}$, $\bar{H}^{(-)}_{\rm eff}$, $\bar{H}^{(+)}_{\rm eff}$, respectively[3] (in fact, it turns out that the spectrum of $\bar{H}_0$ is degenerate if and only if the condition $|\delta| = m\,\nu\,,\ m = 0, 1, 2, \dots\,,$ holds). As a consequence, the evolution operators generated by the effective Hamiltonians $\bar{H}^{(0)}_{\rm eff}$, $\bar{H}^{(-)}_{\rm eff}$,

[2]Namely, a Hamiltonian such that a complete orthonormal set of eigenvectors is given simply by the standard basis $\{|n\rangle \otimes |\pm\rangle\}$.

[3]In correspondence to the resonances (10), the only non-degenerate eigenspaces of $\bar{H}_0$ are given by $\mathrm{span}(|0\rangle \otimes |+\rangle)$, for $\delta = -\nu$, and $\mathrm{span}(|0\rangle \otimes |-\rangle)$, for $\delta = \nu$, that are invariant subspaces for $\bar{H}^{(-)}_{\rm eff}$ and $\bar{H}^{(+)}_{\rm eff}$, respectively. All the other eigenspaces are doubly degenerate.

$\bar{H}^{(+)}_{\text{eff}}$ can be explicitly determined.
Notice moreover that, in particular, $\bar{H}^{(+)}_{\text{eff}}$ — up to a unitary transformation

$$e^{i\pi\,\hat{n}/2}\;\bar{H}^{(+)}_{\text{eff}}\;e^{-i\pi\,\hat{n}/2} = \lambda\,\nu\,\eta\left(a\,\sigma_{+} + \,a^{\dagger}\,\sigma_{-}\right)$$

— has the same form of the typical interaction term of the Jaynes-Cummings Hamiltonian (see ref. [15]).

At this point, it is quite natural to address the following questions:

1. Is it *really* necessary, after having obtained the time-independent Hamiltonian $\bar{H}$, to switch to a further interaction picture in order to achieve a 'good approximate Hamiltonian' — precisely, an effective time-independent interaction picture Hamiltonian such that the associated evolution operator can be explicitly determined — as it is done for applying the RWA?

2. Moreover, does the RWA *really* allow to obtain a correct first order approximation (with respect to the perturbative parameter λ) of the evolution operator?

3. Finally, is it possible to cast in a unique theoretical framework the perturbative treatment of time-independent and time-dependent Hamiltonians in such a way that, for instance, one can study both the time-dependent Hamiltonian $H_0+H_{\updownarrow}(t)$ and the time-independent Hamiltonian $\bar{H}_0 + \bar{H}_{\updownarrow}$ using essentially the same approach (and, hopefully, finding comparable results)?

As it will be seen later on, the answers to these questions (in the respective order) are the following:

1. No, it is not necessary. One can apply a time-independent perturbative approach that allows to obtain approximate expressions of the evolution operator in the remarkable form of a one-parameter group of unitary transformations (see sects. 4 and 6).

2. No, the RWA does not provide, already at the first perturbative order, the correct expression of the evolution operator associated with the Hamiltonian $\bar{H}$;[4] it allows only to reproduce the *qualitative behavior* of the correct first order expression (see sect. 6).

3. Yes. As it will be shown in the subsequent sections, one can develop a suitable perturbative approach that allows to treat on the same footing both time-independent and time-dependent Hamiltonians (see sect. 5). For instance, one can apply this approach to the time-dependent Schrödinger picture Hamiltonian $H_0 + H_{\updownarrow}(t)$ (or $H_0 + H_{\updownarrow}(t)$) and to the time-independent interaction picture Hamiltonian $\bar{H}_0 + \bar{H}_{\updownarrow}$ obtaining the same result, i.e. the same perturbative expansion of the (Schrödinger picture) evolution operator (see sect. 6).

[4]It should be clear that this statement concerns the evolution operator itself and *does not* exclude the possibility that the behavior of certain experimentally observable quantities, with specific initial conditions of the system, may be rather well predicted using the RWA; see the discussion in sect. 7.

3 Basic assumptions and strategy

Let us consider a time-dependent perturbed Hamiltonian $H(\lambda;t)$, namely a selfadjoint linear operator of the form

$$H(\lambda;t) = H_0(t) + H_\diamond(\lambda;t)\,, \tag{14}$$

where $H_0(t)$ is a selfadjoint (and, in general, time-dependent) operator — the 'unperturbed component' — and $H_\diamond(\lambda;t)$ is a time-dependent perturbation; precisely, we will assume that $\lambda \mapsto H_\diamond(\lambda;t)$ is (for the perturbative parameter λ in a certain neighborhood of zero and for any t) a real analytic, selfajoint operator-valued function, with $H_\diamond(0;t) = 0$. A real analytic function can be extended to a domain in the complex plane. Keeping this fact in mind, we will specify that a given property *holds for λ real*. For instance, the analytic function $\lambda \mapsto H_\diamond(\lambda;t)$ will take values in the selfadjoint operators for λ real only.

Let $U(\lambda;t,t_0)$ be the evolution operator associated with $H(\lambda;t)$, with initial time t_0:

$$i\,\dot{U}(\lambda;t,t_0) = H(\lambda;t)\,U(\lambda;t,t_0)\,, \quad U(\lambda;t_0,t_0) = \mathrm{Id}\,, \tag{15}$$

where the dot denotes the time derivative and we have set $\hbar = 1$. Then, we have that

$$U(\lambda;t,t_0) = U_0(t,t_0)\,T(\lambda;t,t_0)\,, \tag{16}$$

where $U_0(t,t_0)$ and $T(\lambda;t,t_0)$ are respectively the evolution operator associated with the unperturbed component $H_0(t)$ (evolution operator which, if the unperturbed Hamiltonian is time-independent, $H_0(t) \equiv H_0$, is obviously given by $e^{-iH_0(t-t_0)}$) and the evolution operator associated with the interaction picture Hamiltonian

$$\tilde{H}(\lambda;t,t_0) := U_0(t_0,t)\,H_\diamond(\lambda;t)\,U_0(t,t_0)\,. \tag{17}$$

Let us notice explicitly that, since $\tilde{H}(0;t,t_0) = 0$, we have:

$$T(0;t,t_0) = \mathrm{Id}\,. \tag{18}$$

We will suppose that the unperturbed evolution $U_0(t,t_0)$ is explicitly known. Then the problem is to determine perturbative expressions of $T(\lambda;t,t_0)$. To this aim, the central point of the paper is the assume for $T(\lambda;t,t_0)$ the following general decomposition:

$$T(\lambda;t,t_0) = \exp\left(-i\,Z(\lambda;t,t_0)\right)\,\exp\left(-i\int_{t_0}^{t} C(\lambda;\mathfrak{t},t_0)\,\mathrm{d}\mathfrak{t}\right)\exp\left(i\,Z(\lambda;t_0,t_0)\right), \tag{19}$$

where $(\lambda;t) \mapsto Z(\lambda;t,t_0)$, $(\lambda;t) \mapsto C(\lambda;t,t_0)$ are operator-valued functions which depend analytically on the perturbative parameter λ; in agreement with condition (18), we set:

$$Z(0;t,t_0) = 0\,, \quad C(0;t,t_0) = 0\,, \quad \forall t\,. \tag{20}$$

We stress that the presence of the term $\exp(i\,Z(\lambda;t_0,t_0))$ in formula (19) ensures that $T(\lambda;t_0,t_0) = \mathrm{Id}$, allowing the possibility that $Z(\lambda;t,t_0) \neq 0$ for $t = t_0$.

It will be seen that decomposition (19) has a wide range of solutions and that a possible choice for fixing a certain class of solutions is given by imposing the condition $C(\lambda;t,t_0)=C(\lambda)$, i.e. assuming that the function $(\lambda;t)\mapsto C(\lambda;t,t_0)$ does not depend on time. This decomposition includes, as particular cases, two decompositions of the evolution operator that have been considered in the literature:

- the decomposition that is obtained setting $Z(\lambda;t,t_0)=0,\ \forall t$, in formula (19), decomposition which is at the root of the *Magnus expansion* of the evolution operator [9];
- the classical *Floquet decomposition* that holds in the case where the interaction picture Hamiltonian depends periodically on time (say with period $\mathtt{T}$) — decomposition which is obtained setting $C(\lambda;t,t_0)\equiv C(\lambda),\quad Z(\lambda;t_0,t_0)=0$, and assuming that $(\lambda,t)\mapsto Z(\lambda;t,t_0)$ is periodic with respect to time with period $\mathtt{T}$ — and that is at the root of the *Floquet-Magnus expansion* of the evolution operator [11].

From this point onwards, for notational convenience, we will fix $t_0=0$. Then, decomposition (19) can be rewritten as

$$T(\lambda;t)=\exp\left(-iZ(\lambda;t)\right)\,\exp\!\left(-i\int_0^t C(\lambda;\mathfrak{t})\,\mathrm{d}\mathfrak{t}\right)\,\exp\left(iZ(\lambda)\right), \tag{21}$$

where: $T(\lambda;t)\equiv T(\lambda;t,0),\ Z(\lambda;t)\equiv Z(\lambda;t,0),\ Z(\lambda)\equiv Z(\lambda;0),\ C(\lambda;t)\equiv C(\lambda;t,0)$. Let us now proceed to obtain perturbative expansions of $C(\lambda;t)$ and $Z(\lambda;t)$. To this aim, if we require the interaction picture evolution operator to satisfy the Schrödinger equation, we get:

$$\begin{aligned}\tilde{H}(\lambda;t)\,T(\lambda;t)\;&=\;i\,\dot{T}(\lambda;t)\\ &=\;e^{-iZ(\lambda;t)}\int_0^1\Big(e^{isZ(\lambda;t)}\,\dot{Z}(\lambda;t)\,e^{-isZ(\lambda;t)}\Big)\mathrm{d}s\;e^{-i\int_0^t C(\lambda;\mathfrak{t})\,\mathrm{d}\mathfrak{t}}e^{iZ(\lambda)}\;+\\ &+\;e^{-iZ(\lambda;t)}\int_0^1\Big(e^{-is\int_0^t C(\lambda;\mathfrak{t})\,\mathrm{d}\mathfrak{t}}\,C(\lambda;t)\,e^{is\int_0^t C(\lambda;\mathfrak{t})\,\mathrm{d}\mathfrak{t}}\Big)\mathrm{d}s\;e^{-i\int_0^t C(\lambda;\mathfrak{t})\,\mathrm{d}\mathfrak{t}}e^{iZ(\lambda)},\end{aligned} \tag{22}$$

where we have used the remarkable formula (see, for instance, ref. [16])

$$\frac{\mathrm{d}}{\mathrm{d}t}\,e^F=e^F\int_0^1\Big(e^{-sF}\,\dot{F}\,e^{sF}\Big)\mathrm{d}s=\int_0^1\Big(e^{sF}\,\dot{F}\,e^{-sF}\Big)\mathrm{d}s\;e^F, \tag{23}$$

which extends to an operator-valued function $t\mapsto F(t)$ the formula for the derivative of the exponential of an ordinary function. Next, let us apply to each member of eq. (22) the operator $e^{iZ(\lambda;t)}$ on the left and the operator $e^{-iZ(\lambda)}e^{i\int_0^t C(\lambda;\mathfrak{t})\,\mathrm{d}\mathfrak{t}}$ on the right:

$$\mathrm{Ad}_{\exp(iZ(\lambda;t))}\,\tilde{H}(\lambda;t)=\int_0^1\Big(\mathrm{Ad}_{\exp(isZ(\lambda;t))}\,\dot{Z}(\lambda;t)+\mathrm{Ad}_{\exp\left(-is\int_0^t C(\lambda;\mathfrak{t})\,\mathrm{d}\mathfrak{t}\right)}\,C(\lambda;t)\Big)\mathrm{d}s\,, \tag{24}$$

where we recall that, given linear operators $\mathfrak{X},Y$, with $\mathfrak{X}$ invertible, $\mathrm{Ad}_{\mathfrak{X}}\,Y:=\mathfrak{X}\,Y\,\mathfrak{X}^{-1}$. Then, since $\mathfrak{X}$ is of the form e^X, we can use the well known relation

$$\mathrm{Ad}_{\exp(X)}\,Y=\exp(\mathrm{ad}_X)\,Y=\sum_{k=0}^{\infty}\frac{1}{k!}\,\mathrm{ad}_X^k\,Y\,, \tag{25}$$

with ad_X^k denoting the k-th power ($\mathrm{ad}_X^0 \equiv \mathrm{Id}$) of the superoperator ad_X defined by $\mathrm{ad}_X Y := [X, Y]$. Eventually, applying formula (25) to eq. (24) and performing the integrals, we obtain:

$$\sum_{k=0}^{\infty} \frac{i^k}{k!} \mathrm{ad}^k_{Z(\lambda;t)} \tilde{H}(\lambda;t) = \sum_{k=0}^{\infty} \frac{i^k}{(k+1)!} \mathrm{ad}^k_{Z(\lambda;t)} \dot{Z}(\lambda;t) + \sum_{k=0}^{\infty} \frac{(-i)^k}{(k+1)!} \mathrm{ad}^k_{\int_0^t C(\lambda;\mathfrak{t})\,\mathrm{d}\mathfrak{t}} C(\lambda;t)\,. \tag{26}$$

This equation will be the starting point for the determination of the operator-valued functions $(\lambda, t) \mapsto Z(\lambda;t)$ and $(\lambda, t) \mapsto C(\lambda;t)$ at each perturbative order in λ, task that will be pursued systematically in the next sections.

4 The time-independent case

We will first consider the most important special case: the case where the Hamiltonian (14) does not depend on time. We have at least three good reasons to single out this case and to study it at the beginning:

- to show that in this case — 'the simplest one' — our perturbative decomposition is far from being trivial;
- to highlight the link between our approach and standard perturbation theory for linear operators, a link that on the other hand is completely missing for Dyson and Magnus expansions;
- to show how this special case can be regarded as a natural starting point for extending the approach to the general time-dependent case ('induction versus deduction').

As it will be clear soon, it will be now convenient to set

$$\mathcal{Z}(\lambda;t) := U_0(t)\, Z(\lambda;t)\, U_0(t)^\dagger, \quad \mathcal{Z}(\lambda) \equiv \mathcal{Z}(\lambda;0) = Z(\lambda)\,, \tag{27}$$

and re-express eq. (26) in terms of the transformed operator $\mathcal{Z}(\lambda;t)$. To this aim, let us first notice that

$$\dot{Z}(\lambda;t) = \mathrm{Ad}_{U_0(t)^\dagger} \Big(\dot{\mathcal{Z}}(\lambda;t) - i\, \mathrm{ad}_{\mathcal{Z}(\lambda;t)} H_0(t) \Big)\,. \tag{28}$$

Besides, given linear operators $\mathfrak{X}$, X and Y, with $\mathfrak{X}$ invertible, one can show easily that

$$\mathrm{ad}^k_{\mathrm{Ad}_{\mathfrak{X}} X} \mathrm{Ad}_{\mathfrak{X}}\, Y = \mathrm{Ad}_{\mathfrak{X}}\, \mathrm{ad}^k_X\, Y, \quad k = 0, 1, 2, \dots\ . \tag{29}$$

Then, since $Z(\lambda;t) = \mathrm{Ad}_{U_0(t)^\dagger}\, \mathcal{Z}(\lambda;t)$, $\tilde{H}(\lambda;t) = \mathrm{Ad}_{U_0(t)^\dagger}\, H_\diamond(\lambda;t)$ and relation (28) holds, using formula (29), from eq. (26) we obtain:

$$\begin{aligned} \mathrm{Ad}_{U_0(t)^\dagger} \sum_{k=0}^{\infty} \frac{i^k}{k!} \mathrm{ad}^k_{\mathcal{Z}(\lambda;t)} H_\diamond(\lambda;t) \;=\; & \mathrm{Ad}_{U_0(t)^\dagger} \Big(\sum_{k=0}^{\infty} \frac{i^k}{(k+1)!} \mathrm{ad}^k_{\mathcal{Z}(\lambda;t)} \dot{\mathcal{Z}}(\lambda;t) \\ & - \sum_{k=1}^{\infty} \frac{i^k}{k!} \mathrm{ad}^k_{\mathcal{Z}(\lambda;t)} H_0(t) \Big) + \sum_{k=0}^{\infty} \frac{(-i)^k}{(k+1)!} \mathrm{ad}^k_{\int_0^t C(\lambda;\mathfrak{t})\,\mathrm{d}\mathfrak{t}} C(\lambda;t). \end{aligned}$$

Next, applying the superoperator $\mathrm{Ad}_{U_0(t)}$ to each member of this equation and rearranging the terms, we get

$$\sum_{k=1}^{\infty} \frac{i^k}{k!} \,\mathrm{ad}^k_{\mathcal{Z}(\lambda;t)}(H_0(t) + H_\diamond(\lambda;t)) + H_\diamond(\lambda;t) \;=\; \mathrm{Ad}_{U_0(t)} \sum_{k=0}^{\infty} \frac{(-i)^k}{(k+1)!} \,\mathrm{ad}^k_{\int_0^t C(\lambda;\mathfrak{t})\,\mathrm{d}\mathfrak{t}}\, C(\lambda;t) + \sum_{k=0}^{\infty} \frac{i^k}{(k+1)!} \,\mathrm{ad}^k_{\mathcal{Z}(\lambda;t)}\, \dot{\mathcal{Z}}(\lambda;t)\,. \tag{30}$$

This equation is, in general, harder to solve than eq. (26); but, in the *time-independent case*, we have that $H_0(t) \equiv H_0$, $H_\diamond(\lambda;t) \equiv H_\diamond(\lambda)$, and it is natural to assume:

$$C(\lambda;t) = C(\lambda)\,, \quad \mathcal{Z}(\lambda;t) = \mathcal{Z}(\lambda;0) = Z(\lambda;0) \equiv Z(\lambda)\,. \tag{31}$$

Then, eq. (30) can be recast in a much simpler form:

$$\sum_{k=1}^{\infty} \frac{i^k}{k!} \,\mathrm{ad}^n_{Z(\lambda)}(H_0 + H_\diamond(\lambda)) + H_\diamond(\lambda) = e^{-iH_0 t}\, C(\lambda)\, e^{iH_0 t}. \tag{32}$$

Now, observe that the first member of this equation does not depend on time, hence the function $t \mapsto e^{-iH_0 t}\, C(\lambda)\, e^{iH_0 t}$ must be constant. It follows that, if we want eq. (32) to be consistent, we have to assume also that $[C(\lambda), H_0] = 0$, i.e. that $C(\lambda)$ *is a constant of the motion for the unperturbed evolution generated by* H_0. Eventually, we find:

$$\sum_{k=1}^{\infty} \frac{i^k}{k!} \,\mathrm{ad}^k_{Z(\lambda)}(H_0 + H_\diamond(\lambda)) + H_\diamond(\lambda) = C(\lambda)\,. \tag{33}$$

At this point, we are ready to obtain perturbative expansions of the operators $C(\lambda)$ and $Z(\lambda)$ (hence, of the interaction picture evolution operator $T(\lambda;t)$). We will suppose that the unperturbed Hamiltonian H_0 has a pure point spectrum, while the case where this hypothesis is not satisfied is a particular case of the general treatment developed in sect. 5. We will denote by $E_1, E_2, \ldots$ the (possibly degenerate) eigenvalues of H_0 and by $P_1, P_2, \ldots$ the associated eigenprojectors. Since the functions $\lambda \mapsto H_\diamond(\lambda)$, $\lambda \mapsto C(\lambda)$ and $\lambda \mapsto Z(\lambda)$ are analytic and $H_\diamond(0) = C(0) = Z(0) = 0$, we can write:

$$H_\diamond(\lambda) = \sum_{n=1}^{\infty} \lambda^n\, H_n\,, \quad C(\lambda) = \sum_{n=1}^{\infty} \lambda^n\, C_n\,, \quad Z(\lambda) = \sum_{n=1}^{\infty} \lambda^n\, Z_n\,. \tag{34}$$

Now, in order to determine the operators $\{C_n\}_{n\in\mathbb{N}}$ and $\{Z_n\}_{n\in\mathbb{N}}$, let us substitute the power expansions (34) in eq. (33); in correspondence to the various orders in the perturbative parameter λ, we get the following set of conditions:

$$C_1 - i\,[Z_1, H_0] - H_1 = 0 \;\;,\;\; [C_1, H_0] = 0 \tag{35}$$

$$C_2 - i\,[Z_2, H_0] + \frac{1}{2}\,[Z_1, [Z_1, H_0]] - i\,[Z_1, H_1] - H_2 = 0 \;\;,\;\; [C_2, H_0] = 0 \tag{36}$$

$$\vdots$$

where we have taken into account the additional constraint $[C(\lambda), H_0] = 0$. This infinite set of equations can be solved recursively and the solution — as it should be expected (we will clarify this point soon) — is not unique. The first equation, together with the first constraint, determines Z_1 up to an operator commuting with H_0 and C_1 uniquely. Indeed, since

$$[C_1, H_0] = 0 \;\Rightarrow\; C_1 = \sum_m P_m\, C_1\, P_m\,, \qquad \text{and} \qquad [Z_1, H_0] = \sum_{j\neq l} (E_l - E_j)\, P_j\, Z_1\, P_l\,, \quad (37)$$

we conclude that

$$C_1 = \sum_m P_m\, H_1\, P_m\,, \qquad \text{and} \qquad Z_1 = \sum_m P_m\, Z_1\, P_m + i \sum_{j\neq l} (E_l - E_j)^{-1}\, P_j\, H_1\, P_l\,. \quad (38)$$

This last equation admits a *minimal solution* which is obtained by imposing a further condition, namely: $P_m\, Z_1\, P_m = 0, \quad m = 1, 2, \dots$.

For $n > 1$, we will adopt an analogous reasoning. Given an operator X, let us set

$$\mathcal{G}_n(X; Z_1, \dots, Z_n) := \sum_{m=1}^{n} \frac{i^m}{m!} \sum_{k_1+\cdots+k_m=n} \mathrm{ad}_{Z_{k_1}} \cdots \mathrm{ad}_{Z_{k_m}} X\,, \quad (39)$$

with $n \geq 1$. Then, for $n \geq 2$, we can define the operator function

$$\mathsf{G}_n(H_0, \dots, H_n; Z_1, \dots, Z_{n-1}) := \sum_{m=0}^{n-1} \mathcal{G}_{n-m}(H_m; Z_1, \dots, Z_{n-m}) - i[Z_n, H_0] + H_n\,. \quad (40)$$

At this point, one can show that the sequence of equations generated by formula (33) is given by

$$\begin{aligned} C_1 - i\,[Z_1, H_0] = H_1 \;\;&,\;\; [C_1, H_0] = 0 \\ &\vdots \\ C_n - i\,[Z_n, H_0] = \mathsf{G}_n(H_0, \dots, H_n; Z_1, \dots, Z_{n-1}) \;\;&,\;\; [C_n, H_0] = 0 \quad n \geq 2 \\ &\vdots \end{aligned} \quad (41)$$

In order to write the general solution of this sequence of equations, it will be convenient to introduce a shorthand notation; given a linear operator X, we set:

$$\langle|X|\rangle_{H_0} := \sum_m P_m\, X\, P_m\,, \quad |\rangle X\langle|_{H_0} := X - \langle|X|\rangle_{H_0} = \sum_{j\neq l} P_j\, X\, P_l\,, \quad (42)$$

$$[|\rangle X\langle|]_{H_0} := i \sum_{j\neq l} (E_l - E_j)^{-1} P_j\, X\, P_l\,. \quad (43)$$

Now, assume that the first n equations have been solved. Then, the operator function $\mathsf{G}_{n+1}(H_0, \dots, H_{n+1}; Z_1, \dots, Z_n)$ is known explicitly and hence

$$C_{n+1} = \langle|\mathsf{G}_{n+1}(H_0, \dots, H_{n+1}; Z_1, \dots, Z_n)|\rangle_{H_0}\,, \quad (44)$$

$$[Z_{n+1}, H_0] = i\,|\rangle \mathsf{G}_{n+1}(H_0, \ldots, H_{n+1}; Z_1, \ldots, Z_n)\langle|_{H_0}\,. \tag{45}$$

Again, this last equation determines Z_{n+1} up to an arbitrary operator $\langle|Z_{n+1}|\rangle_{H_0}$ commuting with H_0; in fact, we have:

$$Z_{n+1} = \langle|Z_{n+1}|\rangle_{H_0} + [|\rangle \mathsf{G}_{n+1}(H_0, \ldots, H_{n+1}; Z_1, \ldots, Z_n)\langle|]_{H_0}\,. \tag{46}$$

We stress that, in general, the choice of a particular solution for Z_{n+1} will also influence the form of $C_{n+2}, Z_{n+2}, \ldots$. Thus, we conclude that the sequence of equations defined above admits infinite solutions (even in the case where H_0 has a non-degenerate spectrum). However, there is a unique *minimal solution* $\{^{\bowtie}C_n, ^{\bowtie}Z_n\}_{n\in\mathbb{N}}$ which fulfills the following additional condition:

$$\langle|^{\bowtie}Z_n|\rangle_{H_0} = 0, \qquad n = 1, 2, \ldots\ . \tag{47}$$

To clarify the link of our approach with standard perturbation theory for linear operators, let us recall a few facts (see [1] [17]). It is possible to show that, under certain technical conditions, there exist positive constants $r_1, r_2, \ldots$ and a simply connected neighborhood $\mathcal{I}$ of zero in $\mathbb{C}$ such that, for any $\lambda \in \mathcal{I}$ and $m = 1, 2, \ldots$, one has that:

1) the following contour integral on the complex plane

$$P_m(\lambda) = \frac{1}{2\pi i} \oint_{\Gamma_m} dz\ \ (z - H(\lambda))^{-1} \tag{48}$$

— where Γ_m is the anticlockwise oriented circle $[0, 2\pi] \ni \theta \mapsto E_m + r_m\, e^{i\theta}$ around the eigenvalue E_m — defines a projection ($P_m(\lambda)^2 = P_m(\lambda)$), which is an orthogonal projection for $\lambda \in \mathcal{I} \cap \mathbb{R}$, with $P_m(0) = P_m$, and $\mathcal{I} \ni \lambda \mapsto P_m(\lambda)$ is an analytic operator-valued function;

2) the range of the projection $P_m(\lambda)$ is an invariant subspace for $H(\lambda)$ (but, if the range of P_m is not 1-dimensional, in general not an eigenspace), hence

$$H(\lambda)\, P_m(\lambda) = P_m(\lambda)\, H(\lambda)\, P_m(\lambda)\,; \tag{49}$$

3) there exists a (non-unique) analytic family $\lambda \mapsto W(\lambda)$ of invertible operators such that

$$P_m = W(\lambda)^{-1} P_m(\lambda)\, W(\lambda)\,, \quad W(0) = \mathrm{Id} \tag{50}$$

— with $W(\lambda)$ unitary for λ real — which is solution of a Cauchy problem of the type $i\,W'(\lambda) = J(\lambda)\, W(\lambda)$, $W(0) = \mathrm{Id}$, where the apex denotes the derivative with respect to the perturbative parameter and $\lambda \mapsto J(\lambda)$ is any analytic family of operators — selfadjoint for λ real — such that

$$\sum_{l\neq m} P_l(\lambda) J(\lambda) P_m(\lambda) = i \sum_m P_m'(\lambda)\, P_m(\lambda) \qquad (*\ P_m(\lambda)\, P_m'(\lambda)\, P_m(\lambda) = 0\ *). \tag{51}$$

In standard (Rayleigh-Schrödinger-Kato) perturbation theory, one can obtain the perturbative corrections to unperturbed eigenvalues and eigenvectors exploiting formula (48) and a suitable expansion of the *resolvent operator* $(z - H(\lambda))^{-1}$ (see, for instance, ref. [18]). In order to recover our previous results, we can use, instead, properties **2)** and **3)** (compare with [2] [6]). Indeed, let us define the operator

$$\overline{H}(\lambda) := W(\lambda)^{-1} H(\lambda)\, W(\lambda)\,, \tag{52}$$

which, for λ real, is unitarily equivalent to $H(\lambda)$. Using relations (49) and (50), we find

$$\overline{H}(\lambda)\, P_m = W(\lambda)^{-1} H(\lambda)\, P_m(\lambda)\, W(\lambda) = W(\lambda)^{-1} P_m(\lambda)\, H(\lambda)\, P_m(\lambda)\, W(\lambda) \tag{53}$$

and hence: $\overline{H}(\lambda)\, P_m = P_m\, \overline{H}(\lambda)\, P_m, \quad m = 1, 2, \dots$. It follows that $\left[\overline{H}(\lambda), H_0\right] = 0$ and then we obtain the following important relation:

$$\left[W(\lambda)^{-1} H(\lambda)\, W(\lambda) - H_0, H_0\right] = 0\,. \tag{54}$$

Thus, if we set $W(\lambda)^{-1} H(\lambda)\, W(\lambda) - H_0 = C(\lambda),\ W(\lambda) = \exp(-i\, Z(\lambda))$, and we apply relation (25), we find precisely eq. (33).

Concluding our treatment of the time-independent case, it is worth stressing that, due to conditions (31), for the overall evolution operator we have:

$$\begin{aligned} U(\lambda; t) &= e^{-iH_0 t}\, e^{-iZ(\lambda;t)}\, e^{-iC(\lambda)t}\, e^{iZ(\lambda)} \\ (*\, \mathcal{Z}(\lambda; t) = e^{-iH_0 t}\, Z(\lambda; t)\, e^{iH_0 t} = Z(\lambda)\, *) \qquad &= e^{-iZ(\lambda)}\, e^{-iH_0 t}\, e^{-iC(\lambda)t}\, e^{iZ(\lambda)} \\ (*\, [C(\lambda), H_0] = 0\, *) \qquad &= e^{-iZ(\lambda)}\, e^{-i(H_0 + C(\lambda))t}\, e^{iZ(\lambda)}, \end{aligned} \tag{55}$$

or, more explicitly,

$$U(\lambda; t) = e^{-iZ(\lambda)} \sum_m \exp(-i(E_m + \lfloor C \rfloor_m(\lambda))t)\, P_m\, e^{iZ(\lambda)}, \tag{56}$$

where we have introduced the *reduced rank operators*

$$\lfloor C \rfloor_m(\lambda) := C(\lambda)\, P_m = P_m\, C(\lambda)\, P_m\,, \quad m = 1, \dots\ . \tag{57}$$

Notice that the truncations at each perturbative order of the expression (56) retain the fundamental property of forming one-parameter groups of unitary transformations. To make this statement precise, let us introduce the following notation. Given an analytic function $\lambda \mapsto f(\lambda) = \sum_{n=0}^{\infty} \lambda^n\, f_n$ and fixed a perturbative order N, we will set

$$f_{[\mathsf{N}]}(\lambda) := \sum_{n=0}^{\mathsf{N}} \lambda^n\, f_n\,; \tag{58}$$

moreover, given another analytic function $\lambda \mapsto h(\lambda)$, we will set:

$$f(\lambda) \overset{\lambda^{\mathsf{N}}}{\approx} h(\lambda) \quad \overset{\text{def}}{\Longleftrightarrow} \quad f_{[\mathsf{N}]}(\lambda) = h_{[\mathsf{N}]}(\lambda)\,. \tag{59}$$

Then, for the evolution operator associated with $H(\lambda;t)$ we have that

$$U(\lambda;t) \overset{\lambda^{\mathsf{N}}}{\approx} \exp(-i\, Z_{[\mathsf{N}]}(\lambda))\, \exp(-i\,(H_0 + C_{[\mathsf{N}]}(\lambda))\, t)\, \exp(i\, Z_{[\mathsf{N}]}(\lambda))\,, \tag{60}$$

where $[C_{[\mathsf{N}]}(\lambda), H_0] = 0$. Thus, the N-th order truncation of our perturbative decomposition of the evolution operator, i.e. the r.h.s. of relation (60), is indeed a one-parameter group of unitary operators.

We conclude this section observing that one can read the array of eqs. (55) 'proceeding from the bottom to the top', namely, one may assume the decomposition

$$U(\lambda;t) = e^{-iZ(\lambda)}\, e^{-i(H_0+C(\lambda))t}\, e^{iZ(\lambda)}, \qquad [C(\lambda), H_0] = 0\,,$$

as a starting point in the case of a time-independent Hamiltonian and induce from this case the general decomposition (21). This is actually the path that has led the author to find the results presented in the paper, extending in a natural way the results previously found in the time-independent case (compare with refs. [2, 3, 4, 5, 6]).

5 The general case

We will now consider eq. (26) in its full generality, equation which can be re-written as

$$\sum_{k=0}^{\infty} \frac{i^k}{k!}\, \mathrm{ad}^k_{Z(\lambda;t)} \left(\tilde{H}(\lambda;t) - \frac{1}{k+1}\, \dot{Z}(\lambda;t) \right) = \mathfrak{C}(\lambda;t)\,, \tag{61}$$

where

$$\mathfrak{C}(\lambda;t) := C(\lambda;t) + \sum_{k=1}^{\infty} \frac{(-i)^k}{(k+1)!}\, \mathrm{ad}^k_{\int_0^t C(\lambda;\mathfrak{t})\, \mathrm{d}\mathfrak{t}}\, C(\lambda;t)\,. \tag{62}$$

The operator $C(\lambda;t)$ can be recovered from the operator $\mathfrak{C}(\lambda;t)$ by means of an order by order procedure. Thus, we can solve eq. (61) for $\mathfrak{C}(\lambda;t)$ up to a given perturbative order and obtain the perturbative expansion of $C(\lambda;t)$ truncated at the same order parallely. Indeed, if we substitute in eq. (62) the power expansions $C(\lambda;t) = \sum_{n=1}^{\infty} \lambda^n\, C_n(t)$ and $\mathfrak{C}(\lambda;t) = \sum_{n=1}^{\infty} \lambda^n\, \mathfrak{C}_n(t)$, and we single out the various perturbative orders, we conclude that the n-th order, which on the l.h.s. is given simply by $\lambda^n\, \mathfrak{C}_n(t)$, consists on the r.h.s. of $\lambda^n\, C_n(t)$ plus a function of $C_1(t), \ldots, C_{n-1}(t)$ and $\int_0^t C_1(\mathfrak{t})\, \mathrm{d}\mathfrak{t}, \ldots, \int_0^t C_{n-1}(\mathfrak{t})\, \mathrm{d}\mathfrak{t}$. Thus, we can achieve an order by order solution. Indeed, one finds out that $C(\lambda;t)$ can be obtained from $\mathfrak{C}(\lambda;t)$ by the following recursive procedure:

$$\begin{aligned}
C_1(t) &= \mathfrak{C}_1(t)\,, \\
&\vdots \\
C_n(t) &= \mathsf{R}_n\left(C_1(t), \ldots, C_{n-1}(t); \int_0^t C_1(\mathfrak{t})\, \mathrm{d}\mathfrak{t}, \ldots, \int_0^t C_{n-1}(\mathfrak{t})\, \mathrm{d}\mathfrak{t} \right) + \mathfrak{C}_n(t)\,, \qquad n \geq 2\,, \\
&\vdots
\end{aligned} \tag{63}$$

where the operator functions $\mathsf{R}_n(\dots)$ are defined as follows. Given linear operators

$$X, X_1, \dots, X_n \quad \text{and} \quad Y_1, \dots, Y_n\,,$$

let us set

$$\mathcal{R}_n(X; Y_1, \dots, Y_n) := -\sum_{m=1}^{n} \frac{(-i)^m}{(m+1)!} \sum_{k_1+\cdots+k_m=n} \mathrm{ad}_{Y_{k_1}} \cdots \mathrm{ad}_{Y_{k_m}} X\,, \quad n \geq 1\,. \tag{64}$$

Then, for $n \geq 2$, we can define the operator function

$$\mathsf{R}_n(X_1, \dots, X_{n-1}; Y_1, \dots, Y_{n-1}) := \sum_{m=1}^{n-1} \mathcal{R}_{n-m}(X_m; Y_1, \dots, Y_{n-m})\,. \tag{65}$$

Let us now investigate the perturbative solutions of eq. (61). Substituting the power expansions $\tilde{H}(\lambda;t) = \sum_{n=1}^{\infty} \lambda^n \tilde{H}_n(t)$, $\mathfrak{C}(\lambda;t) = \sum_{n=1}^{\infty} \lambda^n \mathfrak{C}_n(t)$, $Z(\lambda;t) = \sum_{n=1}^{\infty} \lambda^n Z_n(t)$, we obtain an infinite set of coupled equations that allows to compute order by order the operators $\{\mathfrak{C}_n(t)\}_{n\in\mathbb{N}}$, $\{Z_n(t)\}_{n\in\mathbb{N}}$. In fact, for $n \geq 1$, let us set

$$\breve{\mathcal{G}}_n(X, Y; Z_1, \dots, Z_n) := \sum_{m=1}^{n} \frac{i^m}{m!} \sum_{k_1+\cdots+k_m=n} \mathrm{ad}_{Z_{k_1}} \cdots \mathrm{ad}_{Z_{k_m}} \Big(X - \frac{Y}{m+1} \Big). \tag{66}$$

Then we can define $\breve{\mathsf{G}}_n(\tilde{H}_1(t), \dots, \tilde{H}_n(t); Z_1(t), \dots, Z_{n-1}(t); \dot{Z}_1(t), \dots, \dot{Z}_{n-1}(t))$ as

$$\sum_{m=1}^{n-1} \breve{\mathcal{G}}_{n-m}(\tilde{H}_m(t), \dot{Z}_m(t); Z_1(t), \dots, Z_{n-m}(t)) + \tilde{H}_n(t)\,, \quad n \geq 2\,. \tag{67}$$

With these notations, one can write the sequence of coupled equations which gives a perturbative solution of eq. (61) as follows:

$$\begin{aligned}
\dot{Z}_1(t) &= \tilde{H}_1(t) - \mathfrak{C}_1(\lambda;t)\,, \\
&\vdots \\
\dot{Z}_n(t) &= \breve{\mathsf{G}}_n\Big(\tilde{H}_1(t), \dots, \tilde{H}_n(t); Z_1(t), \dots, Z_{n-1}(t); \dot{Z}_1(t), \dots, \dot{Z}_{n-1}(t)\Big) \\
&\quad - \mathfrak{C}_n(t)\,, \qquad n \geq 2\,, \\
&\vdots
\end{aligned} \tag{68}$$

As in the time-independent case, this infinite set of equations can be solved recursively. Moreover, by virtue of the recursive procedure (63), one can calculate order by order both the operators $\{C_n(t)\}_{n\in\mathbb{N}}$ and $\{Z_n(t)\}_{n\in\mathbb{N}}$. Indeed, integrating with respect to time each equation in the sequence (68) and combining the new sequence of equations so obtained with the recursive process (63), we find

$$\begin{aligned}
Z_1(t) &= \int_0^t \Big(\tilde{H}_1(\mathfrak{t}) - \mathfrak{C}_1(\mathfrak{t}) \Big)\, \mathrm{d}\mathfrak{t} + Z_1\,, \\
C_1(t) &= \mathfrak{C}_1(t)\,,
\end{aligned} \tag{69}$$

at the the first order, and

$$\begin{aligned} Z_2(t) &= \int_0^t \Big(\breve{\mathsf{G}}_2\big(\tilde{H}_1(\mathfrak{t}), \tilde{H}_2(\mathfrak{t}); Z_1(\mathfrak{t}); \dot{Z}_1(\mathfrak{t})\big) - \mathfrak{C}_2(\mathfrak{t}) \Big)\, \mathrm{d}\mathfrak{t} + Z_2 \\ &= \int_0^t \left(i\, \mathrm{ad}_{Z_1(\mathfrak{t})} \left(\tilde{H}_1(\mathfrak{t}) - \frac{1}{2}\, \dot{Z}_1(\mathfrak{t}) \right) + \tilde{H}_2(\mathfrak{t}) - \mathfrak{C}_2(\mathfrak{t}) \right) \mathrm{d}\mathfrak{t} + Z_2\,, \end{aligned}$$

$$\begin{aligned} C_2(t) &= \mathsf{R}_2\left(C_1(t), \int_0^t C_1(\mathfrak{t}) \mathrm{d}\mathfrak{t} \right) + \mathfrak{C}_2(t) \\ &= \frac{i}{2}\, \mathrm{ad}_{\int_0^t C_1(\mathfrak{t}) \mathrm{d}\mathfrak{t}} C_1(t) + \mathfrak{C}_2(t)\,, \\ &\vdots \end{aligned} \tag{70}$$

In general, at the n-th order, for $n \geq 2$, we have:

$$\begin{aligned} Z_n(t) &= \int_0^t \Big(\breve{\mathsf{G}}_n\big(\ldots, \tilde{H}_n(\mathfrak{t}); \ldots, Z_{n-1}(\mathfrak{t}); \ldots, \dot{Z}_{n-1}(\mathfrak{t})\big) - \mathfrak{C}_n(\mathfrak{t}) \Big)\, \mathrm{d}\mathfrak{t} + Z_n\,, \\ C_n(t) &= \mathsf{R}_n\left(\ldots, C_{n-1}(t); \ldots, \int_0^t C_{n-1}(\mathfrak{t})\ \mathrm{d}\mathfrak{t} \right) + \mathfrak{C}_n(t)\,. \end{aligned} \tag{71}$$

Here, differently from the time-independent case, at each perturbative order we have a *couple* of equations. The solution of the first couple (69) is obtained by choosing the arbitrary operator-valued function $t \mapsto \mathfrak{C}_1(t)$ and the arbitrary operator Z_1; similarly, the solution of the n-th couple of equations, for $n \geq 2$, involves the previously computed functions $t \mapsto C_1(t), \ldots, t \mapsto C_{n-1}(t)$, $t \mapsto Z_1(t), \ldots, t \mapsto Z_{n-1}(t)$ and requires the choice of the arbitrary operator-valued function $t \mapsto \mathfrak{C}_n(t)$ and of the arbitrary operator Z_n. *This choice can be fitted according to computational convenience or adapted to specific requirements.*

While the first point (computational advantages) can be best appreciated by means of concrete examples — see sect. 6 — the second one (adapting the solutions to some requirement) will be illustrated considering two important issues. One of these — to characterize the solutions of our perturbative decomposition given a certain class of interaction picture Hamiltonians — will be the subject of last part of the present section. The other one is the following. In many applications it is customary to study a physical system described by an interaction picture Hamiltonian $\tilde{H}(\lambda; t)$ using some effective Hamiltonian $\tilde{E}(\lambda; t)$ which is easier to treat, claiming (usually, on the physical ground) that one can in such a way achieve a satisfactory description of the system. Now, it is natural to address the question:

> *what is the relation, at each perturbative order, between the evolution operator associated with the effective Hamiltonian and the true evolution operator?*

In order to establish a precise setting for this question, we will first provide an interpretation of decomposition (21) which sheds light on its meaning. Notice that this decomposition can be rewritten as

$$T_C(\lambda; t) = T_Z(\lambda; t)^{-1}\, T(\lambda; t)\, T_Z(\lambda; 0), \tag{72}$$

where

$$T_C(\lambda;t) := \exp\!\left(-i\int_0^t C(\lambda;\mathfrak{t})\,\mathrm{d}\mathfrak{t}\right) \quad \text{and} \quad T_Z(\lambda;t) := \exp(-i\,Z(\lambda;t))\,. \tag{73}$$

Formula (72) can be regarded as a passage to a further 'generalized interaction picture' performed on the Hamiltonian $\tilde{H}(\lambda;t)$. Indeed, let us observe that $T_Z(\lambda;t)$ satisfies the equation

$$\begin{aligned} i\,\dot{T}_Z(\lambda;t) &= \mathfrak{Z}_{\mathsf{L}}(\lambda;t)\,T_Z(\lambda;t) \\ &= T_Z(\lambda;t)\,\mathfrak{Z}_{\mathsf{R}}(\lambda;t)\,, \qquad \text{with} \;\; \mathfrak{Z}_{\mathsf{R}}(\lambda;t) = T_Z(\lambda;t)^{-1}\,\mathfrak{Z}_{\mathsf{L}}(\lambda;t)\,T_Z(\lambda;t)\,, \end{aligned} \tag{74}$$

— where $\mathfrak{Z}_{\mathsf{L}}(\lambda;t)$, $\mathfrak{Z}_{\mathsf{R}}(\lambda;t)$ have the following explicit form:

$$\mathfrak{Z}_{\mathsf{L}}(\lambda;t) = \sum_{k=0}^{\infty} \frac{(-i)^k}{(k+1)!}\,\mathrm{ad}^k_{Z(\lambda;t)}\,\dot{Z}(\lambda;t)\,, \qquad \mathfrak{Z}_{\mathsf{R}}(\lambda;t) = \sum_{k=0}^{\infty} \frac{i^k}{(k+1)!}\,\mathrm{ad}^k_{Z(\lambda;t)}\,\dot{Z}(\lambda;t) \tag{75}$$

— or, equivalently, $i\left(\frac{\partial}{\partial t}T_Z^{-1}\right)(\lambda;t) = \mathfrak{Z}_{\mathsf{R}}(\lambda;t)\,T_Z(\lambda;t)^{-1}$. From this relation and eq. (72), one finds that

$$i\,\dot{T}_C(\lambda;t) = \Big(T_Z(\lambda;t)^{-1}\,\tilde{H}(\lambda;t)\,T_Z(\lambda;t) - \mathfrak{Z}_{\mathsf{R}}(\lambda;t)\Big)\,T_C(\lambda;t)\,. \tag{76}$$

Then, by (75) and (76), one can conclude that eq. (61) expresses precisely the fact that $\mathfrak{C}(\lambda;t)$ is the transformed Hamiltonian obtained by switching to this 'new interaction picture'; namely:

$$\mathfrak{C}(\lambda;t) = T_Z(\lambda;t)^{-1}\Big(\tilde{H}(\lambda;t) - \mathfrak{Z}_{\mathsf{L}}(\lambda;t)\Big)\,T_Z(\lambda;t) = T_Z(\lambda;t)^{-1}\,\tilde{H}(\lambda;t)\,T_Z(\lambda;t) - \mathfrak{Z}_{\mathsf{R}}(\lambda;t)\,.$$

It follows that

$$T_C(\lambda;t) = \exp\!\left(-i\sum_{n=1}^{\infty}\lambda^n\int_0^t C_n(\mathfrak{t})\,\mathrm{d}\mathfrak{t}\right) \tag{77}$$

is nothing but the Magnus expansion of the evolution operator associated with the new interaction picture Hamiltonian $\mathfrak{C}(\lambda;t)$.[5]
Hence, coming back to our initial question, it is now clear that, setting $\mathfrak{C}(\lambda;t) = \tilde{E}(\lambda;t)$, decomposition (21) provides precisely an order by order comparison between the true evolution operator $T(\lambda;t)$ and the effective one $T_C(\lambda;t)$ (notice that only the arbitrary constants $\{Z_n\}_{n\in\mathbb{N}}$ are still to be fixed in order to determine the decomposition of $T(\lambda;t)$). A remarkable example of such a comparison will be given in sect. 6.

Let us now turn to the issue of characterizing a certain class of realizations of our perturbative expansion. To classify the whole range of possible solutions and their specific properties would be obviously a problem far beyond the scope of the present paper, in its full generality. Our aim is to study a wide but coherent class of solutions that is particularly relevant for applications.

[5] Again, we stress that we use here the term 'interaction picture' in a generalized sense.

We will first focus on the important class of solutions which is determined by the condition: $\mathfrak{C}_1(t) = \mathfrak{C}_1(0) \equiv \mathfrak{C}_1, \ldots, \mathfrak{C}_n(t) = \mathfrak{C}_n(0) \equiv \mathfrak{C}_n, \ldots \quad \forall t$. This condition is equivalent to the following:

$$C_1(t) = C_1(0) \equiv C_1, \ldots, C_n(t) = C_n(0) \equiv C_n, \ldots \quad \forall t\,. \tag{78}$$

Moreover, if this condition holds, we have: $C_1 = \mathfrak{C}_1, \ldots, C_n = \mathfrak{C}_n, \ldots$. Then the solution of the first equation — namely $Z_1(\{C_1, Z_1\}; t) = \int_0^t \tilde{H}_1(\mathfrak{t})\, \mathrm{d}\mathfrak{t} - t\, C_1 + Z_1$ — is fixed by the choice of the 'arbitrary constants' C_1 and Z_1. Inductively, the solution of the n-th equation can be achieved by substituting the previously obtained solutions $t \mapsto Z_1(\{C_1, Z_1\}, t), \ldots, t \mapsto Z_{n-1}(\{C_k, Z_k\}_{k=1}^{n-1}; t)$ — that are fixed by the choice of the arbitrary constants $C_1, \ldots, C_{n-1}$ and $Z_1, \ldots, Z_{n-1}$ — of the first $n-1$ equations in the formula

$$\begin{aligned} &\vdots \\ Z_n(\{C_k, Z_k\}_{k=1}^n; t) \;=\; &\int_0^t \breve{\mathsf{G}}_n\Big(\ldots; \ldots, Z_{n-1}(\{C_k, Z_k\}_{k=1}^{n-1}; \mathfrak{t}); \ldots, \dot{Z}_{n-1}(\{C_k, Z_k\}_{k=1}^{n-1}; \mathfrak{t})\Big)\mathrm{d}\mathfrak{t} \\ &- t\, C_n + Z_n\,, \qquad n \geq 2\,, \\ &\vdots \end{aligned} \tag{79}$$

which involves the n-th order arbitrary constants C_n and Z_n.
We will now consider a specific possible choice of the arbitrary constants $\{C_n, Z_n\}_{n\in\mathbb{N}}$ up to a certain perturbative order $\mathsf{N} \in \mathbb{N}$. Suppose that the following limits exist (the existence and the meaning of these limits will be investigated presently):

$$\begin{aligned} {}^{\infty}C_1 \;&:=\; \lim_{\tau\to\infty} \frac{1}{\tau}\int_0^\tau \tilde{H}_1(t)\, \mathrm{d}t\,, \\ {}^{\infty}Z_1 \;&:=\; \lim_{\tau\to\infty} \left(-\frac{1}{\tau}\int_0^\tau \left(\int_0^t \left(\tilde{H}_1(\mathfrak{t}) - {}^{\infty}C_1\right)\, \mathrm{d}\mathfrak{t}\right)\, \mathrm{d}t\right) \\ &=\; \lim_{\tau\to\infty} \left(-\frac{1}{\tau}\int_0^\tau \left(\int_0^t \tilde{H}_1(\mathfrak{t})\, \mathrm{d}\mathfrak{t}\right)\mathrm{d}t + \frac{1}{2}\,\tau\, {}^{\infty}C_1\right), \\ &\vdots \\ {}^{\infty}C_{\mathsf{N}} \;&:=\; \lim_{\tau\to\infty} \left(\frac{1}{\tau}\int_0^\tau \breve{\mathsf{G}}_{\mathsf{N}}\Big(\ldots; \ldots; \ldots, \dot{Z}_{\mathsf{N}-1}(\{{}^{\infty}C_k, {}^{\infty}Z_k\}_{k=1}^{\mathsf{N}-1}; t)\Big)\, \mathrm{d}t\right), \\ {}^{\infty}Z_{\mathsf{N}} \;&:=\; \lim_{\tau\to\infty} \left(-\frac{1}{\tau}\int_0^\tau \left(\int_0^t \breve{\mathsf{G}}_{\mathsf{N}}\Big(\ldots; \ldots; \ldots, \dot{Z}_{\mathsf{N}-1}(\{{}^{\infty}C_k, {}^{\infty}Z_k\}_{k=1}^{\mathsf{N}-1}; \mathfrak{t})\Big)\, \mathrm{d}\mathfrak{t}\right)\mathrm{d}t + \frac{1}{2}\,\tau\, {}^{\infty}C_{\mathsf{N}}\right). \end{aligned} \tag{80}$$

Then, one can set $\{C_n = {}^{\infty}C_n,\, Z_n = {}^{\infty}Z_n\}_{n=1}^{\mathsf{N}}$. This particular choice has a remarkable property. Indeed, in the time-independent case — $H_0(t) \equiv H_0$ and $H_\diamond(\lambda; t) \equiv H_\diamond(\lambda)$ — there is a precise relation between the solution associated with the arbitrary constants $\{{}^{\infty}C_n, {}^{\infty}Z_n\}_{n\in\mathbb{N}}$ introduced here and the solutions obtained in sect. 4. As we have done in that section, we will assume that the unperturbed Hamiltonian H_0 has a pure point spectrum. At this point, one can prove that:

1. for any $\mathsf{N} \in \mathbb{N}$, the limits (80) exist;

2. the minimal solution $\{{}^{\bowtie}C_n, {}^{\bowtie}Z_n\}_{n\in\mathbb{N}}$ of the sequence of equations (41), i.e. the solution obtained imposing condition (47), satisfies

$$ {}^{\bowtie}C_n = {}^{\infty}C_n\,, \quad {}^{\bowtie}Z_n = {}^{\infty}Z_n\,, \quad \forall n \in \mathbb{N}\,; \tag{81} $$

3. the solution of the sequence of equations (79) determined by the arbitrary constants $\{{}^{\infty}C_n, {}^{\infty}Z_n\}_{n\in\mathbb{N}}$ is such that

$$ Z_n(\{{}^{\infty}C_k, {}^{\infty}Z_k\}_{k=1}^{n-1}; t) = e^{iH_0 t}\, {}^{\infty}Z_n\, e^{-iH_0 t}, \quad \forall n \in \mathbb{N}\,. \tag{82} $$

Notice that the operators $\{{}^{\infty}C_n, {}^{\infty}Z_n\}_{n\in\mathbb{N}}$ can be calculated by formulae (80) where the eigenprojectors of H_0 — that are involved in the formulae of sect. 4 — do not appear.

We will now prove the existence of the limits (80) (and provide a simple interpretation of their meaning) in two important cases where the (Schrödinger picture) Hamiltonian H of the quantum system is, in general, time-dependent:

- the case where the functions $t \mapsto \tilde{H}_1(t), \ldots$ are periodic;
- the case where the functions $t \mapsto \tilde{H}_1(t), \ldots$ are operator-valued trigonometric polynomials — in the following, for the sake of conciseness, just *trigonometric polynomials* — namely functions of time of the type

$$ F(t) = \sum_{k=1}^{m} A_k\, e^{i\omega_k t}\,, \quad \omega_k \in \mathbb{R}\,, \tag{83} $$

  where $A_1, \ldots, A_m$ are operators in the Hilbert space of our quantum system.

Periodic functions and trigonometric polynomials are examples of *almost-periodic* (a.p.) functions (see [19, 20, 21]).[6] This class of functions has the relevant property of giving rise to a Fourier analysis that generalizes the standard Fourier analysis associated with periodic functions (a generalization mainly due to the great mathematician Harald Bohr). It is worth mentioning that, not only periodic functions, but also trigonometric polynomials play a prominent role among a.p. functions, since any a.p. function can be suitably approximated by a trigonometric polynomial (consider, for instance, the standard Fourier expansion of a periodic function).
Let us recall a few properties that will be useful soon:

(a) for any a.p. function F — in particular, for any periodic function or trigonometric polynomial — one can define the *mean value* $\langle\!\langle\, F \,\rangle\!\rangle$ of F, namely it exists the limit

$$ \langle\!\langle\, F \,\rangle\!\rangle := \lim_{\tau\to\infty} \frac{1}{\tau} \int_0^{\tau} F(t)\, \mathrm{d}t\,; \tag{84} $$

[6] The general definition of a a.p. function is rather technical and will not be used in the following, so we omit it here and we address the reader who may be interested to the cited references. A typical example of a $\mathbb{C}$-valued function which is a.p., but *not* periodic, is provided by the function $t \mapsto (e^{i\varkappa_1 t} + e^{i\varkappa_2 t})$, where $\varkappa_1, \varkappa_2 \in \mathbb{R}$ are such that $\varkappa_1/\varkappa_2$ is irrational.

if F is a periodic function, with period $\mathtt{T}$, one can easily show that $\{\!\{ F \}\!\}$ coincides with the ordinary mean value of F as a periodic function, i.e. $\{\!\{ F \}\!\} = \frac{1}{\mathtt{T}} \int_0^{\mathtt{T}} F(t)\ \mathrm{d}t$; if F is a periodic function with period $\mathtt{T}$ (alternatively, a trigonometric polynomial), then $F - \{\!\{ F \}\!\}$ is a zero-mean-valued periodic function with period $\mathtt{T}$ (respectively, a zero-mean-valued trigonometric polynomial);

(b) given a a.p. function F, if the *primitive*

$$\int F : \mathbb{R} \ni t \mapsto \int_0^t F(\mathfrak{t})\ \mathrm{d}\mathfrak{t} \tag{85}$$

is a a.p. function, then $\{\!\{ F \}\!\} = 0$; in the case where, in particular, F is a periodic function (alternatively, a trigonometric polynomial), the primitive $\int F$ is periodic (respectively, a trigonometric polynomial) if and only if $\{\!\{ F \}\!\} = 0$;

(c) for any a.p. function F, one can define the *essential primitive* of F,[7] namely the function

$$\fint F(t) := \int \big(F - \{\!\{ F \}\!\}\big)(t) = \int_0^t F(\mathfrak{t})\ \mathrm{d}\mathfrak{t} - t\, \{\!\{ F \}\!\}\,; \tag{86}$$

if F is a periodic function with period $\mathtt{T}$, then its essential primitive $\fint F$ is periodic too, with the same period; moreover, the essential primitive of a trigonometric polynomial is still a trigonometric polynomial.

At this point, *we will assume that*

> up to a certain order N, the coefficients $t \mapsto \tilde{H}_1(t), \ldots, t \mapsto \tilde{H}_{\mathsf{N}}(t)$ of the perturbative expansion of the interaction picture Hamiltonian $(\lambda; t) \mapsto \tilde{H}(\lambda; t)$ are periodic functions sharing a common period $\mathtt{T}$, or, alternatively, trigonometric polynomials.

Then, we can show that the limits (80) exist. Indeed, if the function $\tilde{H}_1$ is a periodic function with period $\mathtt{T}$ (alternatively, a trigonometric polynomial), then, by property **(c)**, its essential primitive $\fint \tilde{H}_1$ is a periodic function with the same period (respectively, a trigonometric polynomial). Notice, now, that

$$\begin{aligned} {}^{\infty}C_1 &= \{\!\{ \tilde{H}_1 \}\!\}\,, \\ {}^{\infty}Z_1 &= -\{\!\{ \fint \tilde{H}_1 \}\!\} = -\{\!\{ \int \big(\tilde{H}_1 - \{\!\{ \tilde{H}_1 \}\!\}\big) \}\!\}, \end{aligned} \tag{87}$$

and

$$Z_1(\{{}^{\infty}C_1, {}^{\infty}Z_1\}; t) = \fint \tilde{H}_1(t) - \{\!\{ \fint \tilde{H}_1 \}\!\}\,; \tag{88}$$

hence, $t \mapsto Z_1(\{{}^{\infty}C_1, {}^{\infty}Z_1\}; t)$ is a (zero-mean-valued) periodic function with period $\mathtt{T}$ (respectively, a zero-mean-valued trigonometric polynomial).
Next, if $\mathsf{N} \geq 2$, by this fact and our initial assumption, we find that the function

$$t \mapsto \breve{\mathsf{G}}_2\big(\tilde{H}_1(t), \tilde{H}_2(t); Z_1(\{{}^{\infty}C_1, {}^{\infty}Z_1\}; t); \dot{Z}_1(\{{}^{\infty}C_1, {}^{\infty}Z_1\}; t)\big) \tag{89}$$

[7] This term refers to the idea (typical of signal analysis) that $\fint F$ contains the essential spectral information about F; i.e. that F can be reconstructed from $\fint F$ up to its constant component $\{\!|\, F \,|\!\}$ ('up to a constant offset').

is periodic with period $\mathtt{T}$ (respectively, a trigonometric polynomial) and

$$ {}^{\infty}C_2 = \Big\langle\!\!\Big\langle\, \breve{\mathsf{G}}_2\big(\dots, \tilde{H}_2(\,\cdot\,); \dots; \dot{Z}_1(\{{}^{\infty}C_1, {}^{\infty}Z_1\}; (\,\cdot\,))\big) \,\Big\rangle\!\!\Big\rangle; \tag{90} $$

moreover, by property **(c)**, we have that the essential primitive of the function (89) is periodic with period $\mathtt{T}$ (respectively, a trigonometric polynomial). As a consequence, the limit ${}^{\infty}Z_2$, being (up to a minus sign) the mean value of the essential primitive of the function (89), exists and the function $t \mapsto Z_2(\{{}^{\infty}C_k, {}^{\infty}Z_k\}_{k=1}^{2}; t)$ is periodic with period $\mathtt{T}$ (respectively, a trigonometric polynomial) again.
For $\mathsf{N} \geq 3$ — re-iterating the same argument — one finds out that the limits (80) exist up to the order N. In fact, one finds that, for $2 \leq n \leq \mathsf{N}$, the function

$$ t \mapsto \breve{\mathsf{G}}_n\big(\dots, \tilde{H}_n(t); \dots, Z_{n-1}(\{{}^{\infty}C_k, {}^{\infty}Z_k\}_{k=1}^{n-1}; t); \dots, \dot{Z}_{n-1}(\{{}^{\infty}C_k, {}^{\infty}Z_k\}_{k=1}^{n-1}; t)\big) \tag{91} $$

— together with its essential primitive — is periodic with period $\mathtt{T}$ (respectively, a trigonometric polynomial). Thus, we have:

$$ \begin{aligned} {}^{\infty}C_n &= \Big\langle\!\!\Big\langle\, \breve{\mathsf{G}}_n\big(\dots, \tilde{H}_n(\,\cdot\,); \dots; \dots, \dot{Z}_{n-1}(\{{}^{\infty}C_k, {}^{\infty}Z_k\}_{k=1}^{n-1}; (\,\cdot\,))\big) \,\Big\rangle\!\!\Big\rangle\,, \\ {}^{\infty}Z_n &= -\Big\langle\!\!\Big\langle\, f\breve{\mathsf{G}}_n\big(\dots, \tilde{H}_n(\,\cdot\,); \dots; \dots, \dot{Z}_{n-1}(\{{}^{\infty}C_k, {}^{\infty}Z_k\}_{k=1}^{n-1}; (\,\cdot\,))\big) \,\Big\rangle\!\!\Big\rangle\,, \quad 2 \leq n \leq \mathsf{N}\,; \end{aligned} \tag{92} $$

moreover, for any $2 \leq n \leq \mathsf{N}$, the n-th order solution

$$ \begin{aligned} Z_n(\{{}^{\infty}C_k, {}^{\infty}Z_k\}_{k=1}^{n}; t) \,=\, &\Big(f\breve{\mathsf{G}}_n\big(\dots, \tilde{H}_n(\,\cdot\,); \dots; \dots, \dot{Z}_{n-1}(\{{}^{\infty}C_k, {}^{\infty}Z_k\}_{k=1}^{n-1}; (\,\cdot\,))\big)\Big)(t) \\ &- \Big\langle\!\!\Big\langle\, f\breve{\mathsf{G}}_n\big(\dots, \tilde{H}_n(\,\cdot\,); \dots; \dots, \dot{Z}_{n-1}(\{{}^{\infty}C_k, {}^{\infty}Z_k\}_{k=1}^{n-1}; (\,\cdot\,))\big) \,\Big\rangle\!\!\Big\rangle \end{aligned} \tag{93} $$

is periodic with period $\mathtt{T}$ (respectively, a trigonometric polynomial).

In conclusion, we have shown that

> *if the coefficients $t \mapsto \tilde{H}_1(t), \dots$ of the perturbative expansion of the interaction picture Hamiltonian are periodic functions sharing a common period* $\mathtt{T}$ (alternatively, trigonometric polynomials) *up to a certain order* $\mathsf{N} \geq 1$*, then the limits* (80) *exist, and they are given by formulae* (87) *and* (92)*; moreover, for any $n \leq \mathsf{N}$, the n-th order solution $t \mapsto Z_n(\{{}^{\infty}C_k, {}^{\infty}Z_k\}_{k=1}^{n}; t)$, which is given by formula* (88) *or* (93)*, is a periodic function with period* $\mathtt{T}$ (respectively, a trigonometric polynomial);

in addition, observe that we have the further remarkable property (recall the notation (59) introduced at the end of sect. 4):

> *if the functions $t \mapsto \tilde{H}_1(t), \dots, t \mapsto \tilde{H}_{\mathsf{N}}(t)$ are periodic, sharing a common period* $\mathtt{T}$*, in the* N*-th order approximation of the interaction picture evolution operator*
>
> $$ T(\lambda; t) \overset{\lambda^{\mathsf{N}}}{\approx} \exp(-i\, Z_{[\mathsf{N}]}(\lambda; t))\, \exp(-i\, C_{[\mathsf{N}]}(\lambda)\, t)\, \exp(i\, Z_{[\mathsf{N}]}(\lambda))\,, \tag{94} $$
>
> *where*
>
> $$ Z_{[\mathsf{N}]}(\lambda; t) = \sum_{n=1}^{\mathsf{N}} \lambda^n\, Z_n(\{{}^{\infty}C_k, {}^{\infty}Z_k\}_{k=1}^{n}; t)\,, \tag{95} $$

$$C_{[\mathsf{N}]}(\lambda) = \sum_{n=1}^{\mathsf{N}} \lambda^n \, {}^{\infty}C_n \,, \quad Z_{[\mathsf{N}]}(\lambda) = Z_{[\mathsf{N}]}(\lambda;0) = \sum_{n=1}^{\mathsf{N}} \lambda^n \, {}^{\infty}Z_n \,, \tag{96}$$

the function $\mathbb{R} \ni t \mapsto \exp(-i\, Z_{[\mathsf{N}]}(\lambda;t))$ *is periodic with period* $\mathtt{T}$.

Actually, one can easily prove (along the lines previously drawn) that — in the case where the coefficients $t \mapsto \tilde{H}_1(t), \ldots, t \mapsto \tilde{H}_{\mathsf{N}}(t)$ are periodic functions sharing a common period $\mathtt{T}$ (alternatively, trigonometric polynomials), if at each perturbative order $n \leq \mathsf{N}$ one fixes the operator Z_n *arbitrarily*, and sets $C_1 = \{\!\!\{ \tilde{H}_1 \}\!\!\}$ and, for $\mathsf{N} \geq 2$,[8]

$$C_n = \{\!\!\{ \breve{\mathsf{G}}_n\big(\ldots, \tilde{H}_n(\,\cdot\,); \ldots; \ldots, \dot{Z}_{n-1}(\{C_k, Z_k\}_{k=1}^{n-1}; (\,\cdot\,)) \big) \}\!\!\} \,, \quad 2 \leq n \leq \mathsf{N} \,,$$

so that $Z_1(\{C_1, Z_1\}; t) = \fint \tilde{H}_1(t) + Z_1$ and, for $\mathsf{N} \geq 2$,

$$\begin{aligned} Z_n(\{C_k, Z_k\}_{k=1}^n; t) \;=\; & \Big(\fint \breve{\mathsf{G}}_n\big(\ldots, \tilde{H}_n(\,\cdot\,); \ldots, Z_{n-1}(\{C_k, Z_k\}_{k=1}^{n-1}; (\,\cdot\,)); \ldots \big) \Big)(t) \\ & + \; Z_n \,, \quad 2 \leq n \leq \mathsf{N} \,, \end{aligned} \tag{97}$$

— *the preceding results remain true*; namely: the function $t \mapsto Z_n(\{C_k, Z_k\}_{k=1}^n; t)$, for any $n \in \{1, \ldots, \mathsf{N}\}$, is periodic with period $\mathtt{T}$ (respectively, a trigonometric polynomial). Thus, our perturbative expansion of the evolution operator can indeed be regarded as a generalization of the Floquet-Magnus expansion, which is recovered — in the case where the functions $t \mapsto \tilde{H}_1(t), \ldots, t \mapsto \tilde{H}_{\mathsf{N}}(t)$ are periodic, sharing a common period — by setting in particular: $Z_1 = 0, \ldots, Z_{\mathsf{N}} = 0$.

6 The ion trap Hamiltonian (revisited)

We will now re-consider, in the light of the theory developed in sects. 3, 4 and 5, the quantum Hamiltonian describing a trapped two-level ion interacting with a monochromatic laser field (in the Lamb-Dicke regime). Actually — both for 'pedagogical reasons' and for a wider comparison with the literature on this subject — with respect to sect. 2, we will consider a slightly more general model. As in sect. 2, the Hilbert space of our model is $\mathcal{H}_{\mathrm{F}} \otimes \mathbb{C}^2$ where $\mathcal{H}_{\mathrm{F}}$ is the Fock space, namely a infinite-dimensional Hilbert space endowed with an orthonormal basis $\{|n\rangle : n = 0, 1, \ldots\}$, and with the annihilation and creation operators a, $a^\dagger$ associated with this basis: $a\,|0\rangle = 0$, $a\,|n\rangle = \sqrt{n}\;|n-1\rangle$, $n = 1, 2, \ldots$. The Hamiltonian that we will consider in this section is of the form

$$H(\lambda;t) = H_0 + H_\diamond(\lambda;t) \,, \tag{98}$$

where the unperturbed component H_0, as in sect. 2, is given by[9]

$$H_0 = \nu\, \hat{n} \otimes \mathrm{Id}_{\mathbb{C}^2} + \frac{1}{2}\, \epsilon\, \mathrm{Id}_{\mathcal{H}_{\mathrm{F}}} \otimes \sigma_z \,, \qquad \nu, \epsilon > 0 \tag{99}$$

[8] One can check recursively that the function $t \mapsto \breve{\mathsf{G}}_n\big(\ldots, \tilde{H}_n(t); \ldots; \ldots, \dot{Z}_{n-1}(\{C_k, Z_k\}_{k=1}^{n-1}; t) \big)$ (hence, its essential primitive), for $2 \leq n \leq \mathsf{N}$, is periodic with period $\mathtt{T}$ (respectively, a trigonometric polynomial).

[9] In this section, with respect to sect. 2, we will adopt a somewhat more formal notation that highlights the tensor product structure of our model.

— with $\hat{n}$ and σ_z denoting respectively the number operator $a^\dagger a$, $\hat{n}\,|n\rangle = n\,|n\rangle$, and the effective spin operator (associated with the internal degrees of freedom of the two-level ion) $\sigma_z\,|\pm\rangle = \pm\,|\pm\rangle\,,\ |+\rangle \equiv (1,0)\,,\ |-\rangle \equiv (0,1)$ — while the analytic perturbation $H_\diamond(\lambda;t)$ is now defined by (compare with the interaction term $H_\updownarrow(t)$ defined by (5)):

$$H_\diamond(\lambda;t) := \lambda\nu\Big(e^{i\alpha t}\Big(g(\hat{n}) + e^{i\phi}(a_{_f} + a_{_f}^\dagger)\Big)\otimes\sigma_- + e^{-i\alpha t}\Big(g(\hat{n}) + e^{-i\phi}(a_{_f} + a_{_f}^\dagger)\Big)\otimes\sigma_+\Big), \quad (100)$$

with $\sigma_\pm = |\pm\rangle\,\langle\mp|\,,\ \sigma_+ = \sigma_-^\dagger$ (as usual), with $a_{_f}$ denoting the 'deformed oscillator operator' in $\mathcal{H}_{\rm F}$ defined by

$$a_{_f} := a\,f(\hat{n}) = f(\hat{n}+1)\,a\,, \quad (101)$$

and with the functions $g, f : \{0\}\cup\mathbb{N} \to \mathbb{R}$ (notice that, due to (101), we can set, without loss of generality, $f(0) \equiv 1$) and the phase factor $e^{i\phi}$ characterizing the model. Observe that, since the functions g, f are assumed to be $\mathbb{R}$-valued, we have:

$$g(\hat{n})^\dagger = g(\hat{n})\,, \quad f(\hat{n})^\dagger = f(\hat{n})\,, \quad a_{_f}^\dagger = f(\hat{n})\,a^\dagger = a^\dagger f(\hat{n}+1)\,. \quad (102)$$

Obviously, setting

$$g(n) = 1\,, \quad f(n+1) = \eta\,, \quad \forall n \in \{0\}\cup\mathbb{N}\,, \quad e^{i\phi} = -i\,,$$

we recover the model, with interaction term $H_\updownarrow(t)$, considered in sect. 2; while if we set instead $\epsilon = \nu$, $\alpha = 0$ and $g(n) = 0$, $f(n+1) = \sqrt{n+1}$, $\forall n \in \{0\}\cup\mathbb{N}$, $e^{i\phi} = 1$, we obtain a generalization with 'counter-rotating terms' (i.e. $\lambda\nu\,a_{_f}\otimes\sigma_-$ and $\lambda\nu\,a_{_f}^\dagger\otimes\sigma_+$) of the 'Jaynes-Cummings model with intensity-dependent coupling' studied, for instance, in ref. [22].

Another natural choice of the functions g, f is provided by a more accurate approximation of the interaction term $H_\updownarrow(t)$ of the ion trap Hamiltonian, approximation which is adopted by some authors (see, for instance, refs. [23, 24, 25]). Indeed, it turns out that we have:

$$\begin{aligned} H_\updownarrow(t) \;&=\; \lambda\,\nu\,\big(e^{i\alpha t}\,D(-i\eta)\,\sigma_- + e^{-i\alpha t}\,D(i\eta)\,\sigma_+\big) \\ &=\; \lambda\,\nu\Big(e^{i\alpha t}\,e^{-\eta^2/2}\Big(\Phi_0(\eta;\hat{n}) \\ &+\; \sum_{m=1}^{\infty}(-i\eta)^m\big(\Phi_m(\eta;\hat{n})\,a^m + a^{\dagger m}\Phi_m(\eta;\hat{n})\big)\Big)\otimes\sigma_- +\; h.c.\Big), \end{aligned} \quad (103)$$

where the operator functions $\Phi_0(\eta;\hat{n})$, $\Phi_m(\eta;\hat{n})$, $m = 1, 2, \ldots$, are defined by

$$\Phi_0(\eta;\hat{n}) \;:=\; \sum_{l=0}^{\infty}\frac{(i\,\eta)^{2l}}{(l!)^2}\,(a^\dagger)^l a^l = \sum_{l=0}^{\infty}\frac{(i\,\eta)^{2l}}{(l!)^2}\,[\hat{n}]_l\,, \quad (104)$$

$$\Phi_m(\eta;\hat{n}) \;:=\; \sum_{l=0}^{\infty}\frac{(i\,\eta)^{2l}}{l!\,(l+m)!}\,[\hat{n}]_l\,, \quad (105)$$

with:

$$\begin{aligned} &[n]_0 \equiv 1\,, \quad [n]_l \equiv n\,(n-1)_+\cdots(n-l+1)_+\,, \quad l \geq 1\,, \\ &(n-m)_+ \equiv 0 \quad \text{for } n < m\,, \quad (n-m)_+ \equiv n-m \quad \text{for } n \geq m\,. \end{aligned} \quad (106)$$

Notice that the functions $\{0\} \cup \mathbb{N} \ni n \mapsto \Phi_k(\eta; n),\ k = 0, 1, \dots$, are $\mathbb{R}$-valued.
In order to derive this result, it is sufficient to observe that

$$\begin{aligned} D(\pm i\eta) &:= \exp\Big(\pm i\,\eta\,(a + a^\dagger)\Big) \\ &= e^{-\eta^2/2}\; e^{\pm i\,\eta\,a^\dagger}\; e^{\pm i\,\eta\,a} \\ &= e^{-\eta^2/2}\left(\sum_{l=0}^{\infty} \frac{(i\,\eta)^{2l}}{(l!)^2}\; \overbrace{\underbrace{a^\dagger \cdots a^\dagger}_{l}\; \underbrace{a \cdots a}_{l}}^{[\hat{n}]_l} \right. \\ &\left. \pm\; i\,\eta \sum_{l=0}^{\infty} \frac{(i\,\eta)^{2l}}{l!(l+1)!}\, \big(\underbrace{a^\dagger \cdots a^\dagger}_{l}\; \underbrace{a \cdots a}_{l}\; a + a^\dagger\, \underbrace{a^\dagger \cdots a^\dagger}_{l}\; \underbrace{a \cdots a}_{l} \big) + \cdots \right), \end{aligned} \tag{107}$$

from which formulae (104) and (105) are readily obtained. Notice also that, recalling the expression of the generalized Laguerre polynomial

$$L_n^m(z) = \sum_{l=0}^{n} \binom{n+m}{n-l} \frac{(-z)^l}{l!}\,, \tag{108}$$

we have:

$$\Phi_m(\eta; n) = \frac{n!}{(m+n)!}\, L_n^m(\eta^2)\,, \qquad m, n = 0, 1, 2, \dots\ . \tag{109}$$

Then, in the Lamb-Dicke regime ($\eta \ll 1$), we can set (recall that $f(0) \equiv 1$):

$$g(n) = e^{-\eta^2/2}\, \Phi_0(\eta; n)\,, \quad f(n+1) = \eta\, e^{-\eta^2/2}\, \Phi_1(\eta; n)\,, \quad \forall n \in \{0\} \cup \mathbb{N}\,, \quad e^{i\phi} = -i\,.$$

We are not interested here in performing a complete analysis of the dynamics generated by the Hamiltonian $H(\lambda; t)$, analysis which would involve a careful study of the different regimes associated with specific ranges of the parameters ν, ϵ and α. What is of interest to us is to fix these parameters in such a way that most of the relevant features of our perturbative expansion can be illustrated. We will assume, then, that the parameters ν, α, ϵ satisfy the resonance condition

$$\delta \equiv \epsilon - \alpha = \nu\,, \tag{110}$$

which is also the most interesting regime from the point of view of applications. With condition (110), the interaction picture Hamiltonian has the following expression:

$$\begin{aligned} \tilde{H}(\lambda; t) &= \exp(iH_0 t)\, H_\diamond(\lambda; t)\, \exp(-iH_0 t) \\ &= \lambda\nu\Big(e^{i(\alpha-\epsilon)t}\, g(\hat{n}) \otimes \sigma_- + e^{i\phi}(e^{i(\alpha-\nu-\epsilon)t}\, a_f \otimes \sigma_- + e^{-i(\alpha-\nu+\epsilon)t}\, a_f^\dagger \otimes \sigma_-) + h.c. \Big) \\ &= \lambda\nu\Big(e^{-i\nu t}\, g(\hat{n}) \otimes \sigma_- + e^{i\phi}(e^{-i2\nu t}\, a_f \otimes \sigma_- + a_f^\dagger \otimes \sigma_-) + h.c. \Big)\,. \end{aligned} \tag{111}$$

Notice that it depends periodically on time, with period $\mathtt{T} = 2\pi/\nu$.
At this point, we recall that there is an almost ubiquitous empirical rule in quantum optics, the rotating wave approximation — aimed to drastically simplify the determination of the evolution operator — that says:

"in order to compute the evolution operator, skip the rapidly oscillating terms in the interaction picture Hamiltonian".

This recipe, applied to our case, would lead us to consider for the interaction picture Hamiltonian the following approximation:

$$\tilde{H}(\lambda;t) \approx \lambda\,\nu\,(e^{i\phi}\,a_f^\dagger \otimes \sigma_- + e^{-i\phi}\,a_f \otimes \sigma_+) =: \tilde{E}(\lambda)\,. \tag{112}$$

Clearly, the effective Hamiltonian $\tilde{E}(\lambda)$ — with $f(n) = \eta\,,\ n = 0, 1, \dots$, and $e^{i\phi} = -i$ — coincides with the effective Hamiltonian $\bar{H}^{(+)}_{\text{eff}}$ found in sect. 2. We are going to show that the 'approximation' (112) does not even produce the correct first order expression of the evolution operator.

To obtain the first order perturbative expression of the evolution operator associated with the Hamiltonian $H(\lambda;t)$, we will first exploit the method outlined in sect. 5. To this aim, it will be convenient to introduce the analytic function $\text{avxp} : \mathbb{C} \to \mathbb{C}$, with

$$\text{avxp}(z) = \frac{e^z - 1}{z} \quad \text{for } z \neq 0\,, \quad \text{avxp}(0) = 1\,, \tag{113}$$

and to define, for $\tau > 0$, the operator

$$\begin{aligned} {}^{\tau}C_1 &:= \frac{1}{\lambda\tau}\int_0^\tau \tilde{H}(\lambda;t)\ \mathrm{d}t \\ &= \nu\Big(\text{avxp}(-i\nu\tau)\ g(\hat{n}) \otimes \sigma_- \\ &+ e^{i\phi}\big(\text{avxp}(-i2\nu\tau)\ a_f \otimes \sigma_- + a_f^\dagger \otimes \sigma_-\big) + h.c.\Big)\,. \end{aligned} \tag{114}$$

From this expression, we have immediately (recall formulae (80), and notice that, in this case, $\tilde{H}(\lambda;t) = \lambda\,\tilde{H}_1(t)$) that the operator ${}^{\infty}C_1$ is given by

$${}^{\infty}C_1 = \lim_{\tau\to\infty} {}^{\tau}C_1 = \nu\left(e^{i\phi}\,a_f^\dagger \otimes \sigma_- + e^{-i\phi}\,a_f \otimes \sigma_+\right)\,. \tag{115}$$

Then, we can easily obtain the operator ${}^{\infty}Z_1$:

$$\begin{aligned} {}^{\infty}Z_1 &= \lim_{\tau\to\infty}\left(\frac{1}{2}\tau\,{}^{\infty}C_1 - \frac{1}{\tau}\int_0^\tau t\ {}^{t}C_1\,\mathrm{d}t\right) \\ &= i\,g(\hat{n}) \otimes (\sigma_- - \sigma_+) + \frac{i}{2}\left(e^{i\phi}\,a_f \otimes \sigma_- - e^{-i\phi}\,a_f^\dagger \otimes \sigma_+\right)\,. \end{aligned} \tag{116}$$

Next, the expression of the operator-valued function $t \mapsto Z_1({}^{\infty}C_1, {}^{\infty}Z_1; t)$ is found to be

$$\begin{aligned} Z_1({}^{\infty}C_1, {}^{\infty}Z_1; t) &= {}^{\infty}Z_1 + t\,\big({}^{t}C_1 - {}^{\infty}C_1\big) \\ &= i\,g(\hat{n}) \otimes \big(e^{-i\nu t}\,\sigma_- - e^{i\nu t}\,\sigma_+\big) \\ &+ \frac{i}{2}\left(e^{-i(2\nu t-\phi)}\,a_f \otimes \sigma_- - e^{i(2\nu t-\phi)}\,a_f^\dagger \otimes \sigma_+\right); \end{aligned} \tag{117}$$

hence, it is periodic on time, with the same period $\mathtt{T} = 2\pi/\nu$ of the operator-valued function $t \mapsto \tilde{H}(\lambda;t)$. The reader may verify that the second order contributions can also be

calculated with a rather modest effort.
We notice explicitly that formula (115) shows that the operator $\lambda\,{}^{\infty}C_1$ coincides with the expression of the effective interaction picture Hamiltonian prescribed by the rotating wave approximation, but, due to formulae (116) and (117), this prescription does not provide a correct first order approximate expression of the evolution operator (we will return to this point at the end of the section). Besides, observe that, since ${}^{\infty}Z_1 \neq 0$, we are *not* recovering the Floquet-Magnus expansion.
We stress that we could have obtained this result also by looking for the first order correction to the evolution operator associated with the effective Hamiltonian $\tilde{E}(\lambda)$ — as explained in sect. 5 — with the only additional requirement that the mean value of the function $t \mapsto Z_1({}^{\infty}C_1, {}^{\infty}Z_1; t)$ be zero (condition that fixes the arbitrary constant ${}^{\infty}Z_1$).

Eventually, the unitary operators generated by the selfadjoint operators (115), (116) and (117) can be explicitly computed. Indeed, using the fact that

$$\begin{aligned}\Big(e^{i\theta}\,a_f\otimes\sigma_\pm \pm e^{-i\theta}\,a_f^\dagger\otimes\sigma_\mp\Big)^{2m} &= \Big(\pm\,(a_f^\dagger\,a_f)\otimes(\sigma_\mp\,\sigma_\pm)\pm(a_f\,a_f^\dagger)\otimes(\sigma_\pm\,\sigma_\mp)\Big)^m \\ &= (\pm 1)^m\,\big(\mathsf{f}(\hat{n})^{2m}\,|\mp\rangle\langle\mp| + \mathsf{f}(\hat{n}+1)^{2m}\,|\pm\rangle\langle\pm|\big) \quad (118)\end{aligned}$$

— where we have set, for the sake of notational conciseness,

$$\mathsf{f}(n) := f(n)\sqrt{n} \quad \text{for } n\in\mathbb{N}\,, \quad \mathsf{f}(0)\equiv 1 \tag{119}$$

— we find easily:[10]

$$\begin{aligned}\exp(-i\lambda\,{}^{\infty}C_1\,t) &= \exp\Big(-i\lambda\nu\big(a_f^\dagger\otimes\sigma_- + a_f\otimes\sigma_+\big)\,t\Big) \\ &= \cos\left(\lambda\nu\,\mathsf{f}(\hat{n})\,t\right)\otimes|-\rangle\langle-| + \cos\left(\lambda\nu\,\mathsf{f}(\hat{n}+1)\,t\right)\otimes|+\rangle\langle+| \\ &\quad - i\left(e^{i\phi}\,\frac{\sin\left(\lambda\nu\,\mathsf{f}(\hat{n})\,t\right)}{\mathsf{f}(\hat{n})}\,a_f^\dagger\otimes\sigma_- + e^{-i\phi}\,\frac{\sin\left(\lambda\nu\,\mathsf{f}(\hat{n}+1)\,t\right)}{\mathsf{f}(\hat{n}+1)}\,a_f\otimes\sigma_+\right). \quad (120)\end{aligned}$$

Next, observe that

$$e^{-i\,\lambda\,Z_1({}^{\infty}C_1,{}^{\infty}Z_1;t)} \;\overset{\lambda}{\approx}\; e^{\lambda\,g(\hat{n})\otimes(e^{-i\nu t}\,\sigma_- - e^{i\nu t}\,\sigma_+)}\;e^{\frac{1}{2}\,\lambda\left(e^{-i2\nu t}\,a_f\otimes\sigma_- - e^{i2\nu t}\,a_f^\dagger\otimes\sigma_+\right)}, \tag{121}$$

hence, it will be sufficient to compute the separate exponentials that appear on the r.h.s. of eq. (121). The computation of the first exponential is straightforward:

$$\begin{aligned}e^{\lambda\,g(\hat{n})\otimes(e^{-i\nu t}\,\sigma_- - e^{i\nu t}\,\sigma_+)} &= \cos(\lambda\,g(\hat{n}))\otimes\mathrm{Id}_{\mathbb{C}^2} + \sin(\lambda\,g(\hat{n}))\otimes(e^{-i\nu t}\,\sigma_- - e^{i\nu t}\,\sigma_+) \\ &=: V_{(1)}(\lambda;t)\,. \quad (122)\end{aligned}$$

Then, using again relation (118), we find:

$$\begin{aligned}e^{\frac{1}{2}\,\lambda\left(e^{-i2\nu t}\,a_f\otimes\sigma_- - e^{i2\nu t}\,a_f^\dagger\otimes\sigma_+\right)} &= \cos\left(\tfrac{1}{2}\lambda\,\mathsf{f}(\hat{n}+1)\right)\otimes|-\rangle\langle-| + \cos\left(\tfrac{1}{2}\lambda\,\mathsf{f}(\hat{n})\right)\otimes|+\rangle\langle+| \\ &\quad + \left(e^{-i(2\nu t-\phi)}\,\frac{\sin\left(\frac{1}{2}\lambda\,\mathsf{f}(\hat{n}+1)\right)}{\mathsf{f}(\hat{n}+1)}\,a_f\otimes\sigma_-\right. \\ &\quad \left. - e^{i(2\nu t-\phi)}\,\frac{\sin\left(\frac{1}{2}\lambda\,\mathsf{f}(\hat{n})\right)}{\mathsf{f}(\hat{n})}\,a_f^\dagger\otimes\sigma_+\right) =: V_{(2)}(\lambda;t)\,. \quad (123)\end{aligned}$$

[10] In the following we will set, by convention, $\sin(0)/0 \equiv 1$.

From formulae (122) and (123), we can obtain immediately the expression of $\exp(i\lambda\,{}^{\infty}Z_1)$; indeed:

$$\begin{aligned}\exp(i\lambda\,{}^{\infty}Z_1) &= \exp(i\lambda\,Z_1({}^{\infty}C_1,{}^{\infty}Z_1;0))\\ &\overset{\lambda}{\approx} e^{-\frac{1}{2}\lambda\,(a_f\otimes\sigma_- - a_f^\dagger\otimes\sigma_+)}\;e^{-\lambda\,g(\hat n)\otimes(\sigma_- - \sigma_+)}\\ &= V_{(2)}(\lambda;0)^\dagger\,V_{(1)}(\lambda;0)^\dagger = V_{(2)}(-\lambda;0)\,V_{(1)}(-\lambda;0)\,. \end{aligned}\tag{124}$$

The exponentials above provide a simple explicit form of the first order approximation of the evolution operator:

$$\begin{aligned}T(\lambda;t) &\overset{\lambda}{\approx} \exp(-i\lambda\,Z_1({}^{\infty}C_1,{}^{\infty}Z_1;t))\,\exp(-i\lambda\,{}^{\infty}C_1\,t)\,\exp(i\lambda\,{}^{\infty}Z_1)\\ &\overset{\lambda}{\approx} V_{(1)}(\lambda;t)\,V_{(2)}(\lambda;t)\,\exp(-i\lambda\,{}^{\infty}C_1\,t)\,V_{(2)}(-\lambda;0)\,V_{(1)}(-\lambda;0)\,. \end{aligned}\tag{125}$$

It is worth stressing the non-trivial fact that the action of this operator on the standard basis $\{|n\rangle\otimes|\pm\rangle : n=0,1,\ldots\}$ can be easily computed.

As already observed in sect. 2, a remarkable feature of the time-dependent Hamiltonian $H(\lambda;t)$ is that the associated dynamics can be transformed into the dynamics generated by a time-independent Hamiltonian by switching to a suitable interaction picture, i.e. the interaction picture determined by the reference Hamiltonian $\frac{1}{2}\,\alpha\,\mathrm{Id}_{\mathcal{H}_F}\otimes\sigma_z$. Indeed, setting

$$R_t := \exp\left(-\frac{i}{2}\,\alpha\,\mathrm{Id}_{\mathcal{H}_F}\otimes\,\sigma_z\,t\right),\tag{126}$$

one can define the time-independent 'rotating frame Hamiltonian'

$$\mathfrak{H}(\lambda) := R_t^\dagger\left(H(\lambda;t) - \frac{1}{2}\,\alpha\,\mathrm{Id}_{\mathcal{H}_F}\otimes\,\sigma_z\right)R_t = \mathfrak{H}_0 + \mathfrak{H}_\diamond(\lambda)\,,\tag{127}$$

where (recall relation (110)):

$$\mathfrak{H}_0 := \nu\,\hat n\otimes\mathrm{Id}_{\mathbb{C}^2} + \frac{1}{2}\,(\epsilon-\alpha)\,\mathrm{Id}_{\mathcal{H}_F}\otimes\,\sigma_z = \nu\left(\hat n\otimes\mathrm{Id}_{\mathbb{C}^2} + \frac{1}{2}\,\mathrm{Id}_{\mathcal{H}_F}\otimes\,\sigma_z\right),\tag{128}$$

$$\mathfrak{H}_\diamond(\lambda) := \lambda\,\nu\Big(\Big(g(\hat n) + e^{i\phi}(a_f + a_f^\dagger)\Big)\otimes\,\sigma_- + \Big(g(\hat n) + e^{-i\phi}(a_f + a_f^\dagger)\Big)\otimes\,\sigma_+\Big)\,.\tag{129}$$

We notice explicitly that the further interaction picture Hamiltonian $\tilde{\mathfrak{H}}(\lambda;t)$, obtained from the time-independent Hamiltonian $\mathfrak{H}(\lambda)$ taking as reference Hamiltonian the unperturbed component $\mathfrak{H}_0$, coincides with the 'old' interaction picture Hamiltonian $\tilde H(\lambda;t)$; indeed:

$$\begin{aligned}\tilde{\mathfrak{H}}(\lambda;t) &:= e^{i\mathfrak{H}_0 t}\,\mathfrak{H}_\diamond(\lambda)\,e^{-i\mathfrak{H}_0 t}\\ &= \lambda\nu\Big(e^{-i\nu t}\,g(\hat n)\otimes\,\sigma_- + e^{i\phi}(e^{-i2\nu t}\,a_f\otimes\,\sigma_- + a_f^\dagger\otimes\,\sigma_-) + h.c.\Big)\\ &= \tilde H(\lambda;t)\,. \end{aligned}\tag{130}$$

Hence, we can refer, without ambiguity, to the operators ${}^{\infty}C_1$, ${}^{\infty}Z_1$, and $Z_1({}^{\infty}C_1,{}^{\infty}Z_1;t)$. At this point, the reader may easily verify the following facts:

- using the results of sect. 4, one finds that the operators ${}^{\bowtie}C_1$ and ${}^{\bowtie}Z_1$ coincide respectively with the operators ${}^{\infty}C_1$ and ${}^{\infty}Z_1$ as given by formulae (115) and (116);
- the operator-valued function $t \mapsto Z_1({}^{\infty}C_1, {}^{\infty}Z_1; t)$ satisfies the relation

$$Z_1({}^{\infty}C_1, {}^{\infty}Z_1; t) = e^{i\mathfrak{H}_0 t}\ {}^{\infty}Z_1\ e^{-i\mathfrak{H}_0 t}\,, \tag{131}$$

  in agreement with what has been stated in sect. 5.

The link between the two descriptions — the one associated with the time-dependent Hamiltonian $H(\lambda; t)$ and the one associated with the time-independent Hamiltonian $\mathfrak{H}(\lambda)$ — is given by:

$$\begin{aligned} U(\lambda; t) = R_t\, e^{-i\mathfrak{H}(\lambda)t} &\overset{\lambda}{\approx} R_t\, e^{-i\lambda^{\bowtie}Z_1}\, e^{-i(\mathfrak{H}_0+\lambda^{\bowtie}C_1)t}\, e^{i\lambda^{\bowtie}Z_1} \\ &= R_t\, e^{-i\lambda^{\infty}Z_1}\, e^{-i(\mathfrak{H}_0+\lambda^{\infty}C_1)t}\, e^{i\lambda^{\infty}Z_1} \\ &= R_t\, e^{-i\mathfrak{H}_0 t} \left(e^{i\mathfrak{H}_0 t}\, e^{-i\lambda^{\infty}Z_1}\, e^{-i\mathfrak{H}_0 t} \right) e^{-i\lambda^{\infty}C_1 t}\, e^{i\lambda^{\infty}Z_1} \\ &= e^{-iH_0 t}\, e^{-i\lambda\, Z_1({}^{\infty}C_1, {}^{\infty}Z_1; t)}\, e^{-i\lambda^{\infty}C_1 t}\, e^{i\lambda^{\infty}Z_1} \\ &\overset{\lambda}{\approx} e^{-iH_0 t}\, T(\lambda; t) = U(\lambda; t)\,. \end{aligned}$$

We conclude this section with a final comment. Consider the structure of the first order expression of the evolution operator generated by $\mathfrak{H}(\lambda)$; namely:

$$\exp(-i\mathfrak{H}(\lambda)\, t) \overset{\lambda}{\approx} \underbrace{\exp(-i\lambda^{\infty}Z_1)}_{W(\lambda)}\ \underbrace{\exp(-i(\mathfrak{H}_0 + \lambda^{\infty}C_1)\, t)}_{\mathfrak{R}(\lambda; t)}\ \underbrace{\exp(i\lambda^{\infty}Z_1)}_{W(\lambda)^{\dagger}}.$$

It is then evident that — since $\mathfrak{R}(\lambda; t)$ coincides with the evolution obtained by the RWA — the *true* first order evolution operator can be expressed as the result of the application of a time-independent unitary transformation (associated with the counter-rotating terms) to the RWA evolution. Hence, we can say that the RWA provides at least the first order *qualitative behavior* of the evolution operator associated with $\mathfrak{H}(\lambda)$. On the other hand, observe that

$$\begin{aligned} \exp(-i\mathfrak{H}(\lambda)\, t) &\overset{\lambda}{\approx} W(\lambda)\, \exp(-i\mathfrak{H}_0\, t)\, W(\lambda)^{\dagger}\, \exp(-i\lambda^{\infty}C_1\, t) \\ &= \underbrace{\left(W(\lambda)\, \exp(-i\mathfrak{H}_0\, t)\, W(\lambda)^{\dagger} \exp(i\mathfrak{H}_0\, t)\right)}_{\mathfrak{D}(\lambda; t)}\, \mathfrak{R}(\lambda; t)\,, \end{aligned}$$

where, as it can be easily checked, the operator $\mathfrak{D}(\lambda; t)$ gives a non-trivial first order contribution. Hence, the RWA does not provide, already at the first perturbative order, a correct approximation of the evolution operator associated with $\mathfrak{H}(\lambda)$.
It is also worth observing that the RWA and counter-rotating terms play different roles — but with the same 'dignity' — in the first order approximation provided by our perturbative expansion of the evolution operator.

7 Conclusions and just a glance to further applications

In the present paper, we have introduced a perturbative expansion of the evolution operator associated with a, in general time-dependent, quantum Hamiltonian that exploits the power of the perturbative approach for a twofold purpose:

- to obtain *unitary* approximate expressions of the evolution operator, as in the Magnus expansion, of which it is a generalization;
- simultaneously, to achieve computational advantages, in the same spirit of standard perturbation theory for linear operators.

On our opinion, it is a remarkable fact that the time-independent perturbative approach (essentially, Rayleigh-Schrödinger-Kato perturbation theory) and the time-dependent perturbative approach (Dyson and Magnus expansions) — that are traditionally regarded as completely distinct subjects — can be combined to form such a non-trivial blend. This feature of our perturbative expansion makes it possible, for instance, to treat closely related models — that may be described, depending on the particular case, by a time-independent or by a time-dependent Hamiltonian — using the same general method, so that a direct comparison of the results obtained is achievable.

Remarkable examples of applications of the methods outlined in the present paper are the applications to quantum optical systems. In particular, applications to the study of laser-driven trapped ions (or ions in optical cavities) with various coupling schemes are likely to be very fruitful [2] [5], also in view of the possible implementation, by means of such devices, of quantum computers [26]. For some of these systems, one can switch to a suitable interaction picture to obtain a time-independent effective Hamiltonian, as we have seen in the example studied in sects. 2 and 6, and apply the results of sect. 4. In some other cases, this trick does not work and one can apply the more general results of sect. 5; a simple example is provided by the Hamiltonian describing a trapped ion in interaction with a bichromatic laser field. In all the mentioned cases, the results presented here allow to overcome the severe limitations imposed by the *rotating wave approximation* usually adopted in the literature.

Although a careful criticism of the RWA is not the subject of this paper, it is worth mentioning briefly a few facts. As already observed long time ago by Agarwal [27, 28], who studied spontaneous emission effects in two-level ions, the RWA *should not* be applied directly to the Hamiltonian (hence, for obtaining approximate expressions of the evolution operator), but only — possibly and with due caution — in the calculation of some experimentally observable quantities; if one insists in applying the RWA to the Hamiltonian, the agreement with the 'true' behavior of the experimentally observable quantities can strongly depend both on the choice of the observable itself and on the initial condition of the system. The main point to understand is that the behavior of a single observable quantity does not contain, in general, all the 'information' encoded in the evolution operator.

Several authors have investigated the contribution of the 'counter-rotating terms' in various quantum optical models, contribution which is completely ignored by the RWA; for

instance, perturbative corrections to the energy spectrum [29], and corrections to the time evolution by means of path integral [30], perturbative [31, 32, 33] and numerical [34, 35] techniques have been studied. However, as far as we know, our approach is the first systematic attempt at taking into account the corrections to the RWA evolution operator from a completely general point of view, which allows also to gain a deeper insight in the different roles played by the RWA and counter-rotating terms.

We conclude this section with a final comment. The method introduced in the present paper can be extended in a straightforward way to obtain a perturbative expansion of the *propagator* (or 'evolution family', i.e. the generalization of the unitary evolution operator) associated with a perturbed *evolution equation* in a Banach space (a classical reference on, in general *temporally inhomogeneous* or 'non-autonomous', evolution equations is [36]; see also ref. [37]). Indeed, our method relies on a pure operator approach. This fact implies that it could be applied, in particular, to the study of the dynamics of *open quantum systems* [38, 39, 40, 41], namely, of quantum systems subject to a coupling with an uncontrollable environment or 'bath', coupling that is responsible for the phenomenon known as *quantum decoherence*. Under certain physical conditions, the dynamics of such a system can be described by a propagator whose infinitesimal generator is a 'superoperator' acting on the density operators, i.e. on the positive unit trace operators in the Hilbert space of the quantum system (that form a convex subset of the Banach space of trace class operators). In many important cases (see ref. [41] and the rich bibliography therein), the 'dissipative component' of the superoperator can be considered as (part of) a perturbation, hence, the associated propagator may be expanded using our method.

Acknowledgements

The main results of the paper were presented by the author at the *9-th International Conference on Squeezed States and Uncertainty Relations*, held in Besançon (France), May 2–6, 2005. The author wishes to thank the organizers for the very kind hospitality.

The author wishes to dedicate the present paper, with deep admiration and gratitude, to Prof. F. Zaccaria, a bright example of a scientist and a wonderful person.

References

[1] T. Kato, *Progr. Theor. Phys.* **4**, 514 (1949); T. Kato, *Perturbation Theory for Linear Operators*, Springer-Verlag (1995).

[2] P. Aniello, V. Man'ko, G. Marmo, A. Porzio, S. Solimeno, F. Zaccaria, *J. Russ. Las. Res.* **25**, 30 (2004).

[3] P. Aniello, V. Man'ko, G. Marmo, A. Porzio, S. Solimeno, F. Zaccaria, 'Ion traps in interaction with laser fields: a RWA-free perturbative approach', *Proceedings of the 8-th ICSSUR* (2003).

[4] P. Aniello, V. Man'ko, G. Marmo, A. Porzio, S. Solimeno, F. Zaccaria, *Acta Physica Hungarica B) Quantum Electronics* **20**, 129 (2004).

[5] B. Militello, P. Aniello, A. Messina, *J. Phys. A: Math. Gen.* **37**, 8177 (2004).

[6] P. Aniello, *Int. J. Geom. Meth. Mod. Phys.* **2**, 111 (2005).

[7] F.J. Dyson, *Phys. Rev.* **75**, 486 (1949); *ibidem*, 1736.

[8] P. Pechukas, J.C. Light, *J. Chem. Phys.* **44**, 3897 (1966).

[9] W. Magnus, *Commun. Pure Appl. Math.* **7**, 649 (1954).

[10] P.C. Moan, J.A. Oteo, *J. Math. Phys.* **42**, 501 (2001).

[11] F. Casas, J.A. Oteo, J. Ros, *J. Phys. A: Math. Gen.* **34**, 3379 (2001).

[12] A. Galindo, M.A. Martin-Delgado, *Rev. Mod. Phys.* **74**, 347 (2002).

[13] J.I. Cirac, A.S. Parkins, R. Blatt, P. Zoller, *Adv. At. Mol. Opt. Phys.* **37**, 237 (1996).

[14] W.P. Schleich, *Quantum Optics in Phase Space*, WILEY-VCH (2001).

[15] E.T. Jaynes, F.W. Cummings, Proc. IEEE **51**, 89 (1963).

[16] R.M. Wilcox, *J. Math. Phys.* **8**, 962 (1967).

[17] M. Reed, B. Simon, *Methods of Modern Mathematical Physics* IV, Academic Press (1978).

[18] A. Messiah, *Quantum Mechanics* II, North-Holland (1986).

[19] H. Bohr, *Almost Periodic Functions*, Chelsea Publishing Company (1951).

[20] L. Amerio, G. Prouse, *Almost Periodic Functions and Functional Equations*, Van Nostrand Reinhold (1971).

[21] S. Zaidman, *Almost Periodic Functions in Abstract Spaces*, Pitman (1985).

[22] M. Chaichian, D. Ellinas, P. Kulish, *Phis. Rev. Lett.* **65**, 980 (1990).

[23] C.A. Blockey, D.F. Walls, H. Risken, *Europhys. Lett.* **17**, 509 (1992).

[24] R.L. de Matos Filho, W. Vogel, *Phys. Rev. A* **50**, R1988 (1994).

[25] W. Vogel, R.L. de Matos Filho, *Phys. Rev. A* **52**, 4214 (1995).

[26] M.A. Nielsen, I.L. Chuang, *Quantum Computation and Quantum Information*, Cambridge University Press (2000).

[27] G.S. Agarwal, *Phys. Rev. A* **4**, 1778 (1971).

[28] G.S. Agarwal, *Phys. Rev. A* **7**, 1195 (1973).

[29] C. Cohen-Tannoudji, J. Dupont-Roc, C. Fabre, *J. Phys. B* **6**, L214 (1973).

[30] K. Zaheer, M.S. Zubairy, *Phys. Rev. A* **37**, 1628 (1988).

[31] R. Vyas, S. Singh, *Phys. Rev. A*, **33**, 375 (1986).

[32] S.J.D. Phoenix, *J. Mod. Opt.* **38**, 695 (1991).

[33] Mao-Fa Fang, Peng Zhou, *J. Mod. Opt.* **42**, 1199 (1995).

[34] J. Seke, *Quant. Opt.* **3**, 127 (1991).

[35] G. Berlin, J. Aliaga, *J. Opt. B: Quant. Semiclass. Opt.* **6**, 231 (2004).

[36] K. Yosida, *Functional Analysis*, Grund. Math. Wiss. vol. 123, Springer-Verlag (1968).

[37] K.J. Engel, R. Nagel, *One-parameter Semigroups for Linear Evolution Equations*, GTM vol. 194, Springer (2000).

[38] V. Gorini, A. Kossakowski, E.C.G. Sudarshan, *J. Math. Phys.* **17**, 821 (1976).

[39] G. Lindblad, *Comm. Math. Phys.* **48**, 119 (1976).

[40] A.S. Holevo, *Statistical Structure of Quantum Theory*, Lecture Notes in Physics vol. m 67, Springer (2001).

[41] H.P. Breuer, F. Petruccione, *The Theory of Open Quantum Systems*, Oxford University Press (2002).